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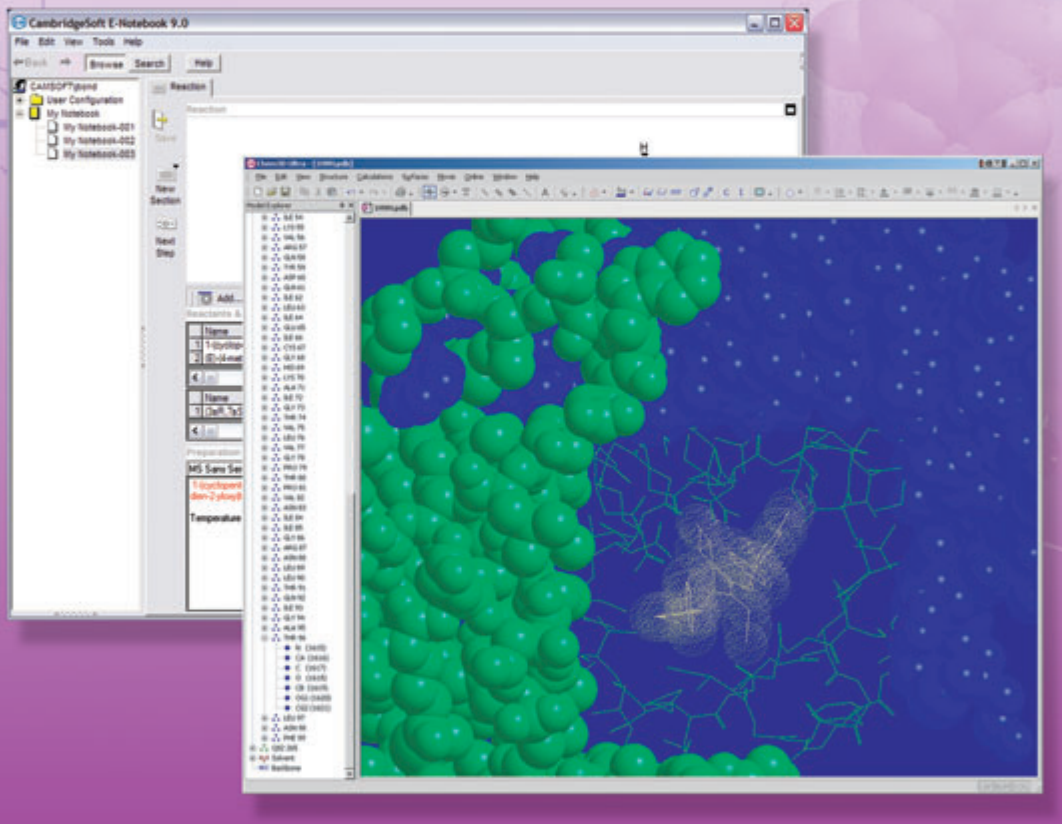

ChemOffice®

Chem3D, ChemFinder and E-Notebook

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User's Guide

Revision 9.0.1
12/22/04

CS *Chem3D* 9.0

for Windows

***Chem3D* is a stand alone application within**

***ChemOffice*, an integrated suite including**

***ChemDraw* for Chemical Structure Drawing**
***ChemFinder* for searching and information integration,**
***BioAssay* for biological data retrieval and visualization,**
***Inventory* for managing and searching reagents,**
***E-Notebook* for electronic journal and information, and**
***ChemInfo* for chemical and reference databases.**

Chem3D®

Molecular Modeling and Analysis Standard

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Q: That makes sense, but what do I get out of purchasing my own software?

A: When you purchase authorized copies of software programs, you receive user guides and tutorials, quick reference cards, the opportunity to purchase upgrades, and technical support from the software publishers. For most software programs, you can read about user benefits in the registration brochure or upgrade flyer in the product box.

Q: What exactly does the law say about copying software?

A: The law says that anyone who purchases a copy of software has the right to load that copy onto a single computer and to make another copy "for archival purposes only" or, in limited circumstances, for "purposes only of maintenance or repair." It is illegal to use that software on more than one computer or to make or distribute copies of that software for any other purpose unless specific permission has been obtained from the copyright owner. If you pirate software, you may face not only a civil suit for damages and other relief, but criminal liability as well, including fines and jail terms of up to one year

Q: So I'm never allowed to copy software for any other reason?

A: That's correct. Other than copying the software you purchase onto a single computer and making another copy "for archival purposes only" or "purposes only of maintenance or repair," the copyright law prohibits you from making additional copies of the software for any other reason unless you obtain the permission of the software company.

Q: At my company, we pass disks around all the time. We all assume that this must be okay since it was the company that purchased the software in the first place.

A: Many employees don't realize that corporations are bound by the copyright laws, just like everyone else. Such conduct exposes the company (and possibly the persons involved) to liability for copyright infringement. Consequently, more and more corporations concerned about their liability have written policies against such "softlifting". Employees may face disciplinary action if they make extra copies of the company's software for use at home or on additional computers within the office. A good rule to remember is that there must be one authorized copy of a software product for every computer upon which it is run

Q: Can I take a piece of software owned by my company and install it on my personal computer at home if instructed by my supervisor?

A: A good rule of thumb to follow is one software package per computer, unless the terms of the license agreement allow for multiple use of the program. But some software publishers' licenses allow for "remote" or "home" use of their software. If you travel or telecommute, you may be permitted to copy your software onto a second machine for use when you are not at your office computer. Check the license carefully to see if you are allowed to do this.

Q: What should I do if become aware of a company that is not compliant with the copyright law or its software licenses?

A: Cases of retail, corporate and Internet piracy or non-compliance with software licenses can be reported on the Internet at http://www.siia.net/piracy/report.asp or by calling the Anti-Piracy Hotline: (800) 388-7478.

Q: Do the same rules apply to bulletin boards and user groups? I always thought that the reason they got together was to share software.

A: Yes. Bulletin boards and user groups are bound by the copyright law just as individuals and corporations. However, to the extent they offer shareware or public domain software, this is a perfectly acceptable practice. Similarly, some software companies offer bulletin boards and user groups special demonstration versions of their products, which in some instances may be copied. In any event, it is the responsibility of the bulletin board operator or user group to respect copyright law and to ensure that it is not used as a vehicle for unauthorized copying or distribution.

Q: I'll bet most of the people who copy software don't even know that they're breaking the law.

A: Because the software industry is relatively new, and because copying software is so easy, many people are either unaware of the laws governing software use or choose to ignore them. It is the responsibility of each and every software user to understand and adhere to copyright law. Ignorance of the law is no excuse. If you are part of an organization, see what you an do to initiate a policy statement that everyone respects. Also, suggest that your management consider conducting a software audit. Finally, as an individual, help spread the word that users should be "software legal."

Q: What are the penalties for copyright infringement?

A: The Copyright Act allows a copyright owner to recover monetary damages measured either by: (1) its actual damages plus any additional profits of the infringer attributable to the infringement, or (2) statutory damages, of up to $150,000 for each copyrighted work infringed. The copyright owner also has the right to permanently enjoin an infringer from engaging in further infringing activities and may be awarded costs and attorneys' fees. The law also permits destruction or other reasonable disposition of all infringing copies and devices by which infringing copies have been made or used in violation of the copyright owner's exclusive rights. In cases of willful infringement, criminal penalties may also be assessed against the infringer.

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"Don't Copy that Floppy" video
This 9 minute rap video, available for $10, is designed to educate students on the ethical use of software.

Other education materials including, "Software Use and the Law", a brochure detailing the copyright law and how software should be used by educational institutions, corporations and individuals; and several posters to help emphasize the message that unauthorized copying of software is illegal.

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	Includes	Manuals	ChemDraw Chemical Structure Drawing Standard	ChemOffice Chem3D, ChemFinder & E-Notebook	ChemOffice Enterprise Solutions And Databases
Software	ChemDraw		■		
	Chem3D			■	
	ChemFinder			■	
	E-Notebook Desktop			■	
	Inventory Desktop				■
	BioAssay Desktop				■
Desktop Applications	ChemDraw/Excel		■		
	ChemFinder/Office			■	
	CombiChem/Excel			■	
	ChemSAR/Excel			■	
	MOPAC, MM2			■	
	CS Gaussian, GAMESS Interface			■	
Enterprise Solutions	ChemOffice WebServer				■
	Oracle Cartridge				■
	E-Notebook Workgroup, Enterprise			■	
	Document Manager				■
	Registration Enterprise				■
	Formulations & Mixtures				■
	Inventory Workgroup, Enterprise				■
	Discovery LIMS				■
	BioAssay Workgroup, Enterprise				■
	BioSAR Enterprise				■
	ChemDraw/Spotfire				■
Databases	The Merck Index				■
	ChemACX, ChemSCX				■
	ChemMSDX				■
	ChemINDEX, NCI & AIDS				■
	ChemRXN				■
	Ashgate Drugs				■
Tips	Structure Drawing Tips		■		
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Introduction

About Chem3D

Chem3D is an application designed to enable scientists to model chemicals. It combines powerful building, analysis, and computational tools with a easy-to-use graphical user interface, and a powerful scripting interface.

Chem3D provides computational tools based on molecular mechanics for optimizing models, conformational searching, molecular dynamics, and calculating single point energies for molecules.

About CS MOPAC

CS MOPAC is an implementation of the well known semi-empirical modeling application MOPAC, which takes advantage of the easy-to-use interface of Chem3D. CS MOPAC currently supports MOPAC 2002.

There are two CS MOPAC options available with Chem3D 9.0.1:

- MOPAC Ultra
- MOPAC Pro

MOPAC Ultra is the full MOPAC implementation, and is only available as an optional addin. The CS MOPAC Ultra implementation provides support for previously unavailable features such as MOZYME and PM5 methods.

MOPAC Pro allows you to compute properties, perform simple (and some advanced) energy minimizations, optimize to transition states, and compute properties. The CS MOPAC Pro implementation supports MOPAC sparkles, has an improved user interface, and provides faster calculations. It is included in some versions of Chem3D, or may be purchased as an optional addin. Contact CambridgeSoft sales or your local reseller for details.

CAUTION

If you have CS MOPAC installed on your computer from a previous Chem3D or ChemOffice installation, upgrading to version 9.0.1 will remove your existing MOPAC installation. See the ReadMe for instructions on saving your existing MOPAC menu extensions.

See Chapter 10, "MOPAC Computations" on page 165 for more information on using CS MOPAC.

About Gaussian

Gaussian is a cluster of programs for performing semi-empirical and *ab initio* molecular orbital (MO) calculations. Gaussian is not included with CS Chem3D, but is available from SciStore.com, http://scistore.cambridgesoft.com/software/ .

When Gaussian is correctly installed, Chem3D communicates with it and serves as a graphical front end for Gaussian's text-based input and output.

Chem3D is compatible with Gaussian 03 for Windows, and requires the 32-bit version.

About CS Mechanics

CS Mechanics is an add-in module for Chem3D. It provides three force-fields—MM2, MM3, and MM3 (Proteins)—and several optimizers that allow for more controlled molecular mechanics calculations. The default optimizer used is the Truncated-Newton-Raphson method, which

provides a balance between speed and accuracy. Other methods are provided that are either fast and less accurate, or slow but more accurate.

What's New in Chem3D 9.0?

Chem3D 9.0 is enhanced by the following features:

- **Redesigned GUI**—User customizable, with new toolbars, new layout for tables and subviews, new menus and dialogs. The GUI has been redesigned from the ground up to make it more usable.
- **New Model Hierarchy Tree Control**—Lets you open and close fragments, chains, or groups; change display properties at different levels. See "Working With the Model Explorer" on page 111.
- **ChemDraw panel**—Building small molecules is easier than ever. See "Building with the ChemDraw Panel" on page 74.
- **New menu organization**—Important functions are easier to locate.
- **Full screen mode**—Use Chem3D for demos or instruction.
- **New Dihedral Driver**—Do conformation analysis with graphical display of results. See "Tutorial 5: Mapping Conformations with the Dihedral Driver" on page 42.
- **Improved support for small molecule overlays**—compare different conformations or different structures. See "Tutorial 6: Overlaying Models" on page 43.
- **XML table editor**—easier to use, better integration.

What's New in Chem3D 9.0.1?

- **View translation tool—**translate (pan) the view without changing the model coordinates. See "Moving Models with the Translate Tool" on page 96.
- **Safer viewing**—new "pure selection tool" prevents unintentionally moving or rotating parts of the model while selecting. See "The Building Toolbar" on page 20.
- **Global keyboard modifiers**—advanced users can perform any action while in any mode using a global keyboard modifier. See "Keyboard Modifiers" on page 235.
- **Improved Zoom control**—zoom to center of screen, center of selection, or center of rotation. See "Zoom and Translate" on page 235.
- **Display axes**—display or hide axes centered at the origin of the model, or at the origin of the view focus.
- **Middle mouse button and scroll wheel support**—use scroll wheel to zoom, middle mouse button to rotate or translate. See entries under "Rotation" and "Zoom and Translate" on page 235.
- **New tools for large models:**
  - **View focus**—selects a subset of the model for viewing and manipulation. See "View Focus" on page 85.
  - **Select higher group**—double click a selection to select the next higher group. See "Selecting a Group or Fragment" on page 93.
  - **Radial Selection**—select atoms or groups within a specified radius. See "Selecting Atoms or Groups by Distance" on page 94.

For Users of Previous Versions of Chem3D

Many features have changed in Chem3D 9.0. Please note the following:

- The rotation bars are now dynamic rather than permanently displayed. See "Rotation Bars" on page 14 for details.
- Internal rotations have changed. See "Rotating Models" on page 96 for details on how to perform internal rotations.
- The Measurements table has been augmented by three other tables: the Model Explorer, the Cartesian Coordinates table, and the Z-Matrix table. See "The Model Explorer" on page 27, and "Model Coordinates" on page 28for more details.
- Menus and toolbars have changed. Consult the relevant sections of the manual for details.

CambridgeSoft Web Pages

The following table contains the addresses of ChemDraw-related web pages.

For information about ...	Access ...
Technical Support	http://www.cambridgesoft.com/services
ChemDraw Plugin	http://products.cambridgesoft.com/ProdInfo.cfm?pid=278 http://products.cambridgesoft.com/ProdInfo.cfm?pid=279
Software Developer's kit	http://sdk.cambridgesoft.com/
ActiveX control	http://sdk.cambridgesoft.com/
Purchasing CambridgeSoft products and chemicals	http://chemstore.cambridgesoft.com/

Installation and System Requirements

Before installation, see the "ReadMeFirst" and any other ReadMe documents on the installation CD-ROM.

Microsoft®Windows® Requirements

- Windows 2000 or XP.
- Microsoft® Excel add-ins require Office 2000, 2003, or XP.
- ChemDraw plugins/ActiveX® controls support Netscape® 6.2.x and 7.x, Mozilla 1.x, and Microsoft IE 5.5 SP2 and 6.x. The Chem3D ActiveX control supports IE 5.5 SP2 and 6.x *only*. There is no Chem3D plugin available.

NOTE: *Windows XP Service Pack 2 includes security features that automatically block active content. This means that by default, Internet Explorer blocks ChemDraw and Chem3D ActiveX controls. To activate them, you must choose the option to "allow blocked content" from the bar appearing under the address bar notifying you that the security settings have blocked some of the content of the page. IE does not remember this information, so you must repeat*

the activation each time you access the page. If you visit a site frequently, you can add it to the list of trusted sites in IE's security settings.

- Screen resolution must be 800 x 600 or higher.

Site License Network Installation Instructions

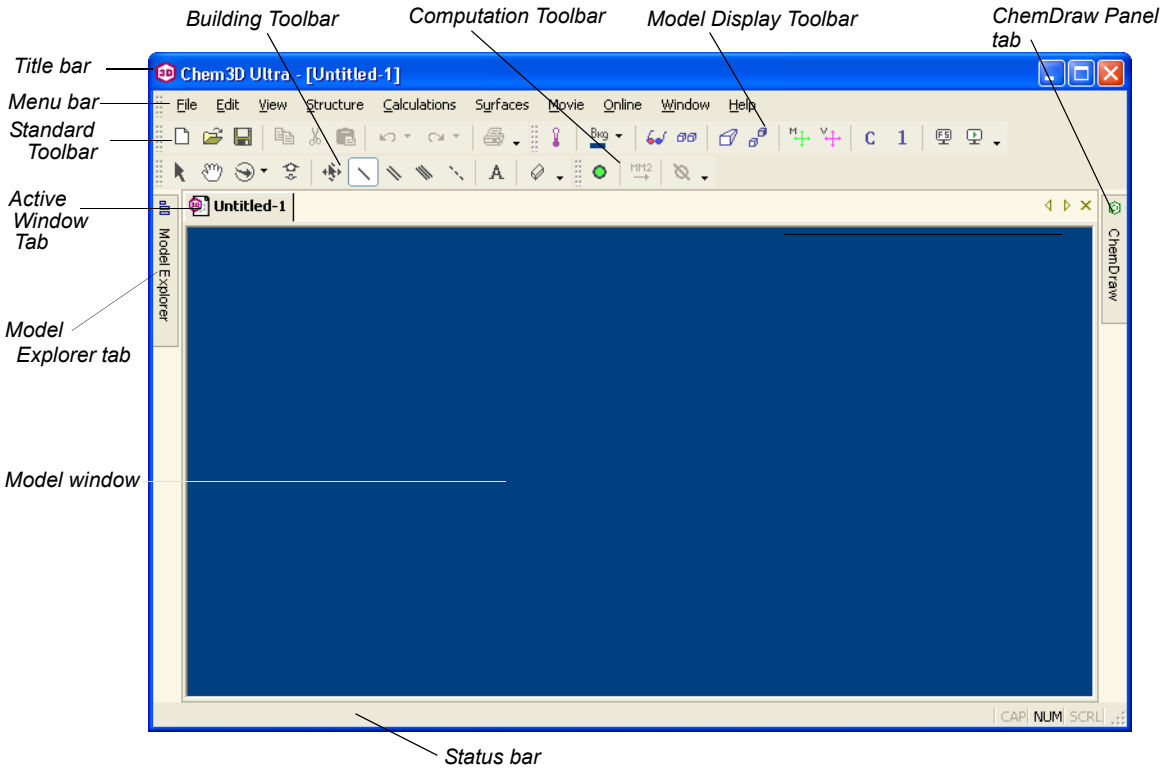
If you have purchased a site license, please see the following web site for network installation instructions:

http://www.cambridgesoft.com/services/sl/

Chapter 1: Chem3D Basics

The Graphical User Interface

The Graphical User Interface (GUI) is the part of Chem3D that you interact with to perform tasks. The GUI consists of a model window, menus, toolbars and dialog boxes. It can also include up to three optional panels that display Output and Comments boxes, the Model Explorer and tables (Cartesian coordinates, Z-Matrix, and Measurement), and the ChemDraw Panel. At the bottom of the GUI is a Status bar which displays information about the active frame of your model and about hidden atoms in your model. The GUI is shown in Rotation mode with the dynamic Rotation bars showing, the ChemDraw panel open, and the Tables panel set to Auto-Hide.



Model Window

The Model window is the work space where you do your modeling. If there is textual information about the model, it appears in the Output window or the Status bar.

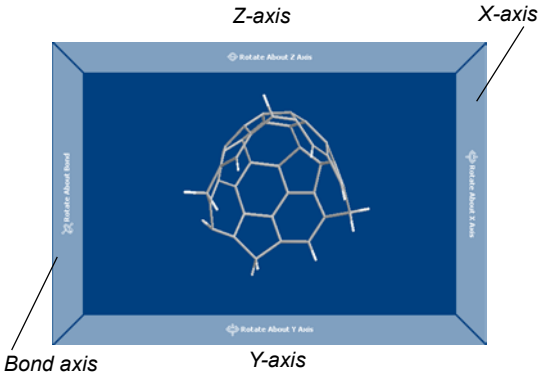
The following table describes the objects in the Model window.

Object	Description
Model area	The workspace where a molecular model is viewed, built, edited, or analyzed. The origin of the Cartesian axes (0,0,0) is always located at the center of this window, regardless of how the model is moved or scaled. The Cartesian axes do not move relative to the window.
Active Window tab	Chem3D 9 can open multiple models simultaneously. The tab selects the active window.

Rotation Bars

Chem3D 9 introduces dynamic (auto-hide) rotation bars. The rotation bars only appear on your screen when you are actually using them. To view the dynamic rotation bars you must do two things:

- Activate rotation mode by selecting the Trackball tool.
- "Mouse over" the rotation bar area.



Click on a bar and drag to rotate a model around that axis. The "Rotate About a Bond" bar is only active when a bond or dihedral is selected. Freehand rotation is accomplished by dragging in the main window. The cursor changes to a hand when you are in freehand rotation mode.

You can turn off the display (but not the function) of the bars with the Show Mouse Rotation Zones checkbox on the GUI tab of the Preferences dialog box (File > Preferences).

Menus and Toolbars

All Chem3D commands and functions can be accessed from the menus or toolbars. The toolbars contain icons that offer shortcuts to many commonly used functions. You can activate the Toolbars you want from the Toolbars submenu of the View menu.

Toolbars can be attached to any side of the GUI, or can be "torn off" and placed anywhere on the screen for convenience.

TIP: *Most Toolbar commands are duplicated from the menus, and are intended as a convenience. If you only use a command infrequently, you can save clutter by using the menu commands.*

The File Menu

In addition to the usual File commands, you use the File menu to access the Chem3D Templates and Preferences, and the Model Settings.

- **Import File—**Import MOL2 and SD files into Chem3D a document. The import utility accurately preserves model coordinates.
- **Model Settings**—Displays the Settings dialog box. Set defaults for display modes and colors, model building, atom and ligand display, atom labels and fonts, movie and stereo pair settings, and atom/bond popup label information.

- **Preferences**—Displays the Preferences dialog box. Set defaults for image export, calculation output path, OpenGL settings and including hydrogens in CDX format files.
- **Sample Files**—Accesses example models.

The Edit Menu

In addition to the usual Edit functions, you can use the Edit menu to copy the model in different formats, to clear the model window, and to select all or part of the model.

- **Copy as**—Puts the model on the Clipboard in ChemDraw format, as a SMILES string, or in bitmap format.
- **Copy As ChemDraw Structure**—Puts the model on the Clipboard in CDX format. You may only paste the structure into an application that can accept this format, for example ChemDraw, ChemFinder, or Chem3D.
- **Copy As SMILES**—Puts the model on the Clipboard as a SMILES string. You may only paste the structure into an application that can accept this format.
- **Copy As Picture**—Puts the model on the Clipboard as a bitmap. You may only paste the structure into an application that can accept bitmaps.

NOTE: *The application you paste into must recognize the format. For example, you cannot paste a ChemDraw structure into a Microsoft Word document.*

- **Paste Special**—Preserves coordinates when pasting a Chem3D model from one document to another.
- **Clear**—Clears the model window of all structures.
- **Select All**—Selects the entire model.
- **Select Fragment**—If you have selected an atom, selects the fragment that atom belongs to.

The View Menu/Model Display Toolbar

Use the View menu to select the view position and focus, as well as which toolbars, tables, and panels are visible. The Model Display submenu of the View menu duplicates all of the commands in the Model Display toolbar.

- **View Position**—The View Position submenu gives you options for centering the view, fitting the window, and aligning the view with an axis.
- **View Focus**—The View Focus submenus is used to set the focus. See "View Focus" on page 85
- **Model Display**—Duplicates the Model Display toolbar—Contains tools to control the display of the model. These tools are duplicated on the View menu..
  - **Show Atom Labels**—A toggle switch to display or hide the atom labels.
  - **Show Serial Numbers**—A toggle switch to display or hide the atom numbers.
  - **Show Atom Dots**—Displays or hides atom dot surfaces for the model. The dot surface is based on VDW radius or Partial Charges, as set in the Atom Display table of the Settings dialog box.
  - **Show Atom Spheres**—Displays or hides atom spheres for the model. The radius is based on VDW radius or Partial Charges, as set in the Atom Display table of the Settings dialog box.
  - **Show Hs and Lps**—A toggle switch to display or hide hydrogen atoms and lone pairs.
  - **Red and Blue glasses**—A toggle switch to set the display for optimal viewing with red-blue 3D glasses to create a stereo effect.

- **Stereo Pairs**—A toggle switch to enhance three dimensional effect by displaying a model with two slightly different orientations. It can also create orthogonal (simultaneous front and side) views. The degree of separation is set on the Stereo View tab of the Settings dialog box.
- **Perspective**—A toggle switch to create a perspective rendering of the model by consistent scaling of bond lengths and atom sizes by depth. The degree of scaling is controlled by the Perspective "Field of View" slider on the Model Display tab of the Settings dialog box.
- **Depth Fading**—A toggle switch to create a realistic depth effect, where more distant parts of the model fade into the background. The degree of fading is controlled by the Depth Fading "Field of View" slider on the Model Display tab of the Settings dialog box.
- **Model Axes**—Displays or hides the Model axes.
- **View Axes**—Displays or hides the view axes.

NOTE: *When both axes overlap and the Model axes are displayed, the View axes are not visible.*

- **Background Color**—Displays the Background color select toolbar. Dark backgrounds are best for viewing protein ribbon or cartoon displays. Selecting red-blue or Chromatek 3D display will automatically override the background color to display the optimal black background. Background colors are not used when printing, except for Ribbon displays. When saving a model as a GIF file, the background will be transparent, if you have selected that option for Image Export in the Preferences dialog box.
- **Color By**—Selects the model coloring scheme. See "Coloring Displays" on page 58 for more information.

- **Toolbars**—Click the name of a toolbar to select it for display. Click again to deselect. You can attach a toolbar to any side of the GUI by dragging it to where you want it attached. If you are using a floating toolbar, you can change its shape by dragging any of its edges.
  - **Standard toolbar**—Contains standard file, edit, and print tools. The commands are duplicated on the File and Edit menus.
  - **Building toolbar**—Contains the Select, Translate, Rotate, and Zoom tools in addition to the model building tools—bonds, text building tool, and eraser. These tools are **not** duplicated on any menu. This toolbar is divided into "safe" and "unsafe" tools. The four "safe" tools on the left control only the view – they do not affect the model in any way. This includes the new "safe" select tool and the new translate tool . The old select tool is now called the Move tool. Although it can also be used to select, it's primary use is to move atoms and fragments.
  - **Model Display toolbar**—Contains tools to control the display of the model. These tools are duplicated on the View menu.
  - **Surfaces toolbar**—Contains tools to calculate and display a molecular surface. Molecular Surface displays provide information about entire molecules, as opposed to the atom and bond information provided by Structure displays.
  - **Movies toolbar**—Contains tools for the creation and playback of movies. Chem3D movies are animations of certain visualization operations, such as iterations from a computation. They can be viewed in

Chem3D, or saved in Windows AVI movie format. The commands are reproduced on the Movie menu.

- **Calculation toolbar**—Performs MM2 minimization from a desktop icon. The spinning- arrow icon shows when any calculation is running, and the Stop icon can be used to stop a calculation before it's preset termination.
- **Status bar**—Displays the Status bar, which displays information about the active frame of your model.
- **Customize**—Displays the Customize dialog box. Customizing toolbars is a standard MS Windows operation, and is not described in Chem3D documentation.

- **Model Explorer**—Displays a hierarchical tree representation of the model. Most useful when working with complex molecules such as proteins, the Model Explorer gives you highly granular control over the model display.
- **ChemDraw Panel**—Displays the ChemDraw Panel. Use the ChemDraw Panel to build molecules quickly and easily with familiar ChemDraw drawing tools. You can import, export, edit, or create small molecules quickly and easily using the ChemDraw ActiveX tools palette.
- **Cartesian Table**—Displays the Cartesian Coordinates table. Cartesian Coordinates describe atomic position in terms of X-, Y-, and Z-coordinates relative to an arbitrary origin.
- **Z-Matrix Table**—Displays the internal coordinates, or Z-Matrix, table. Internal coordinates are the most commonly used coordinates for preparing a model for further computation.
- **Measurements Table**—Displays the Measurements table.The Measurements table displays bond lengths, bond angles, dihedral angles, and ring closures.
- **Parameters Tables**—Displays a list of external tables that are used by Chem3D to construct models, perform computations and display results.
- **Output Box**—Displays the Output box, which presents textual information about the model, iterations, etc.
- **Comments Box**—Displays the Comments box, a place for user comments that is stored with the file.
- **Dihedral Chart**—Opens the window displaying results of Dihedral Driver MM2 computation. See "Tutorial 5: Mapping Conformations with the Dihedral Driver" on page 42 for more information.
- **Status Bar**—Displays or hides the Status Bar.
- **Start Spinning Model Demo**—Spins the model on the Y axis. Use stop calculation on the Calculations toolbar to stop the demo.
- **Full Screen**—Activates the full screen display.

The Structure Menu

The Structure menu commands populate the Measurements table and control movement of the model.

The Measurements submenu

- **Set… Measurements**—Sets a measurement—bond length, angle, or distance—according to what is selected.
- **Bond Lengths**—Displays bond lengths in the Measurements Table. The Actual values come from the model and the Optimal values come from the Bond Stretching Parameters external table.

- **Bond Angles**—Displays bond angles in the Measurements Table. The **Actual** values come from the model and the **Optimal** values come from **Angle Bending Parameters** and other external tables.
- **Dihedral Angles**—Displays dihedral angles in the Measurements Table. The **Actual** values come from the model and the **Optimal** values come from **Angle Bending Parameters** and other external tables.
- **Clear**—Clears the entire Measurement table. If you only want to clear part of the table, select the portion you want to clear, and choose **Delete** from the right-click menu.

The Model Position submenu

- **Center Model on Origin**—Resizes and centers the model in the model window after a change to the model is made.
- **Center Selection on Origin**—Resizes and centers the selected portion of the model in the model window.
- **Align Model With X Axis**—When two atoms are selected, moves them to the X-axis.
- **Align Model With Y-axis**—When two atoms are selected, moves them to the Y-axis.
- **Align Model With Z-axis**—When two atoms are selected, moves them to the Z-axis.
- **Align Model With XY Plane**—When three atoms are selected, moves them to the XY-plane.
- **Align Model With XZ Plane**—When three atoms are selected, moves them to the XZ-plane.
- **Align Model With YZ Plane**—When three atoms are selected, moves them to the YZ-plane.

The Reflect Model submenu

- **Through XY Plane**—Reflects the model through the XY plane by negating Z coordinates. If the model contains any chiral centers this will change the model into its enantiomer. Pro-R positioned atoms will become Pro-S and Pro-S positioned atoms will become Pro-R. All dihedral angles used to position atoms will also be negated.
- **Through XZ Plane**—Reflects the model through the XZ plane by negating Y coordinates. If the model contains any chiral centers this will change the model into its enantiomer. Pro-R positioned atoms will become Pro-S and Pro-S positioned atoms will become Pro-R. All dihedral angles used to position atoms will also be negated.
- **Through YZ Plane**—Reflects the model through the YZ plane by negating X coordinates. If the model contains any chiral centers this will change the model into its enantiomer. Pro-R positioned atoms will become Pro-S and Pro-S positioned atoms will become Pro-R. All dihedral angles used to position atoms will also be negated.
- **Invert Through Origin**—Reflects the model through the origin, negating all Cartesian coordinates. If the model contains any chiral centers this will change the model into its enantiomer. Pro-R positioned atoms will become Pro-S and Pro-S positioned atoms will become Pro-R. All dihedral angles used to position atoms will also be negated.

The Set Z-Matrix submenu

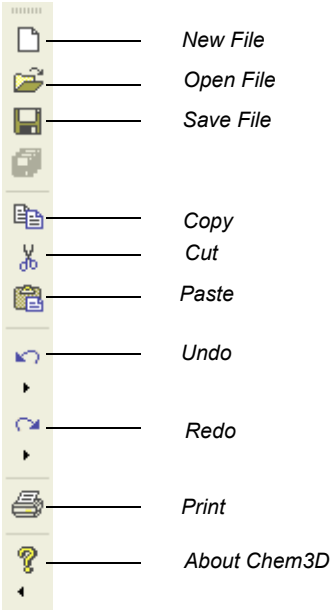
- **Set Origin Atom(s) file**—Sets the selected atom(s) as the origin of the internal coordinates. Up to three atoms may be selected. "Setting Measurements" on page 85

- **Position by Dihedrals**—Positions an atom relative to three previously positioned atoms using a bond distance, a bond angle, and a dihedral angle. For more information on changing the internal coordinates see "Setting Dihedral Angles" on page 86.
- **Position by Bond Angles**—Positions an atom relative to three previously positioned atoms using a bond distance and two bond angles. For more information on changing the internal coordinates see "Setting Bond Angles" on page 86.

- **Detect Stereochemistry**—Scans the model and lists the stereocenters in the Output box.
- **Invert**—Inverts the isomeric form. For example, to invert a model from the *cis*- form to the *trans*- form, select one of the stereo centers and use the Invert command.
- **Deviation from Plane**—When you select four or more atoms, outputs the RMS deviation from the plane to the Output window.
- **Add Centroid**—Adds a centroid to a selected model or fragment. At least two atoms must be selected. The centroid and "bonds" to the selected atoms are displayed, and "bond" lengths can be viewed in the tool tips. To delete a centroid, select it and press the Delete or Backspace key.
- **Rectify**—Fills the open valences for an atom, usually with hydrogen atoms. This command is only useful if the default automatic rectification is turned off in the **Model Settings** dialog box.
- **Clean Up**—Corrects unrealistic bond lengths and bond angles that may occur when building models, especially when you build strained ring systems.
- **Overlay**—The Overlay submenu provides all of the commands to enable you to compare fragments by superimposing one fragment in a model window over a second fragment. Two types of overlay are possible: quick, and minimization. See "Tutorial 6: Overlaying Models" on page 43, and "Comparing Models by Overlay" on page 109 for information on each overlay type.
- **Dock**—The Dock command enables you to position a fragment into a desired orientation and proximity relative to a second fragment. Each fragment remains rigid during the docking computation.

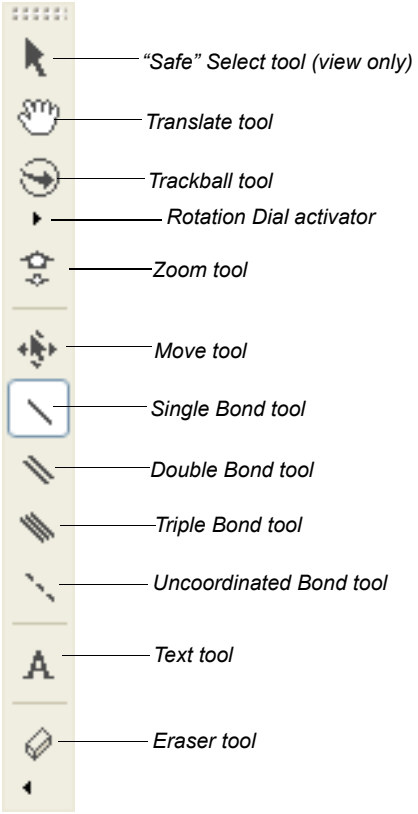
The Standard Toolbar

The Standard toolbar contains tools for standard Windows functions, including up to 20 steps of Undo and Redo.

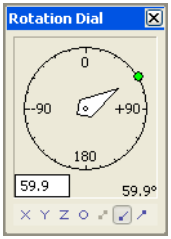


The Building Toolbar

The Building toolbar contains tools that allow you to create and manipulate models. The tools are shown below.



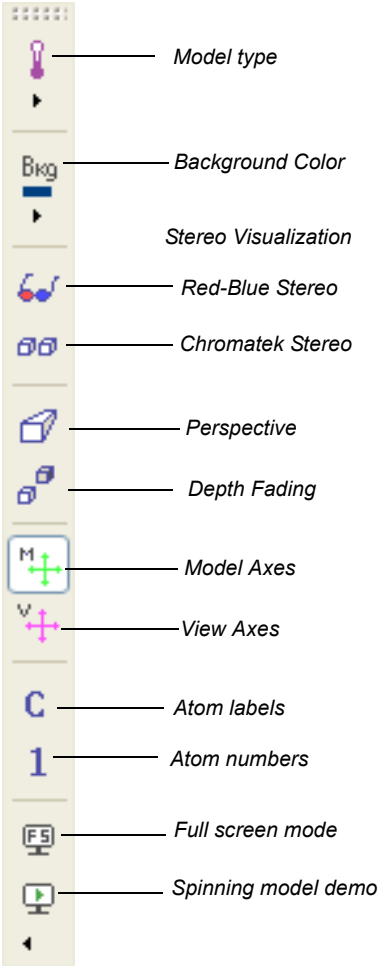
The Rotation Dial, activated by clicking the arrow under the Trackball tool, lets you rotate a model an exact amount. Select an axis, then drag the dial or type a number into the box.



For detailed descriptions of the tools see "Building With the Bond Tools" on page 75, "Rotating Models" on page 96, and "Resizing Models" on page 100.

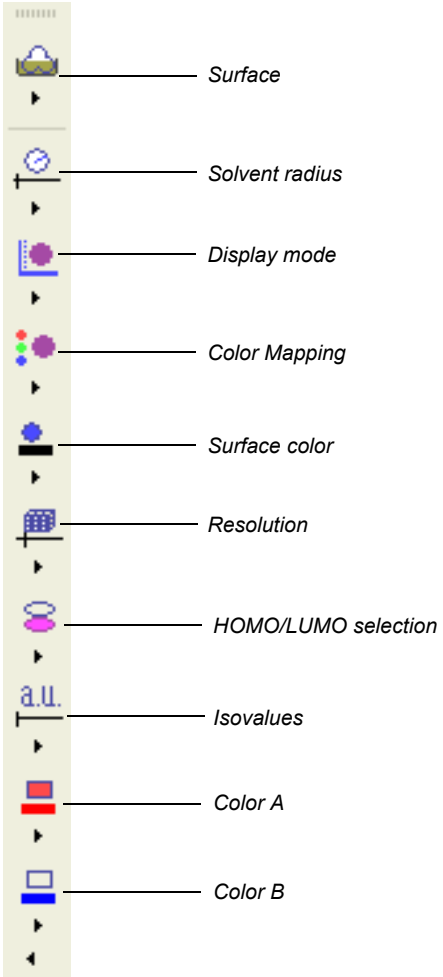
The Model Display Toolbar

The Model Display toolbar contains tools for all of the Chem3D display functions. The Model type and Background color tools activate menus that let you choose one of the options. All of the remaining tools are toggle switches—click once to activate; click again to deactivate.



The Surfaces Toolbar

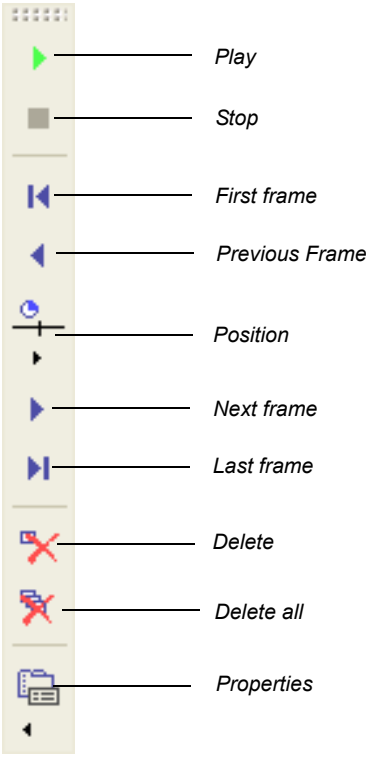
The Surfaces toolbar controls the display of molecular surfaces. In most cases, you will need to do either an Extended Hückel, MOPAC, or Gaussian calculation before you can display surfaces.



For more information on Surfaces, see "Molecular Surface Displays" on page 63.

The Movie Toolbar

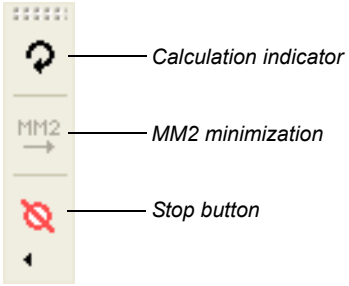
The Movie toolbar controls the creation and playback of animations. You can animate certain visualization operations, such as iterations from a computation, by saving frames in a movie. Movies can be saved as Windows AVI video files.



For more information on Movies, see "Creating and Playing Movies" on page 115.

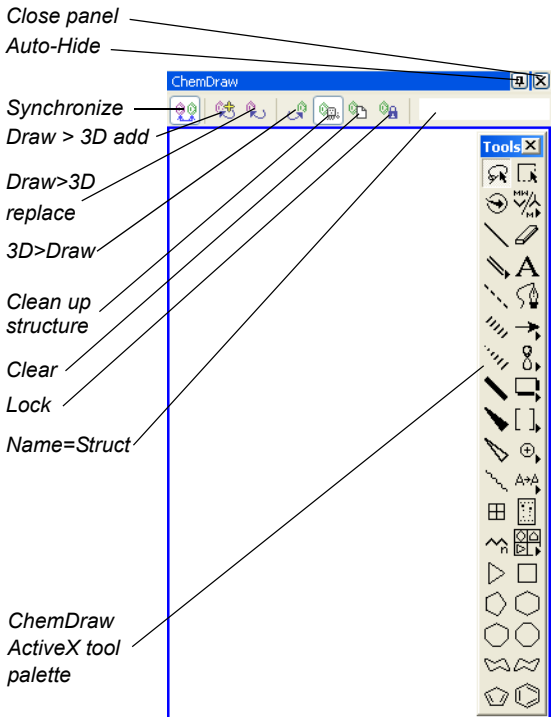
The Calculation Toolbar

The Calculation toolbar provides a desktop icon for performing the most common calculation, MM2 minimization. It also provides a Stop button and a "calculation running" indicator that work with all calculations.



The ChemDraw Panel

Chem3D 9 makes it easier than ever to create or edit models in ChemDraw. The ChemDraw panel is activated from the View menu. By default it opens on the right side of the GUI, but like the toolbars you can have it "float" or attach it anywhere you like.



Use the 3D > Draw icon to drag a Chem3D model into the ChemDraw panel.

To create a model in ChemDraw, click in the ChemDraw panel to activate the ChemDraw toolbar. Use the Draw>3D Add or Draw>3D Replace icons to put the model in Chem3D—or select the Synchronize icon to draw in both simultaneously. You can also create a model by typing the name of a compound—or a SMILES string—into the *Name=Struct*™ box. When you finish editing, add or replace your Chem3D model by clicking the appropriate icon.

The Model Information Panel

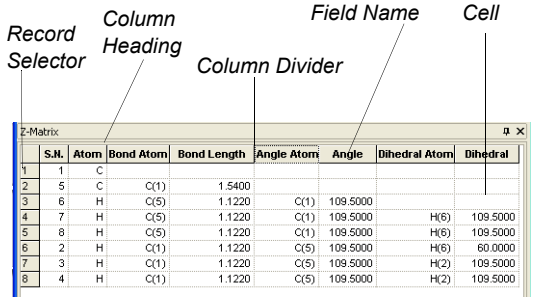
The Model information panel contains information about the model in the top-most tabbed window and its display. You can display one or more of the following tables in the area:

- Model Explorer
- Measurements
- Cartesian Coordinates
- Z-Matrix table

Tables are linked to the structure so that selecting an atom, bond, or angle in either will highlight both. Numerical values in the tables can be edited or cut and pasted to/from other documents (text or Excel worksheets), and the changes are displayed in the structure.

All of the tables have an Auto-hide feature to minimize their display. For more information on Model Tables, see "Model Coordinates" on page 28.

The Z-Matrix table is shown below:



The following table describes the elements of the Measurement table.

Table Element	Description
Column Heading	Contains field names describing the information in the table.
Record Selector	Used to select an entire record. Clicking a record selector highlights the corresponding atoms in the model window.
Field Name	Identifies the type of information in the cells with which it is associated.
Column Divider	Used to change the width of the column by dragging.
Cell	Contains one value of one field in a record. All records in a given table contain the same number of cells.

The Output and Comments Windows

The Output and Comments boxes are typically found at the bottom of the GUI window. You can have them float if you wish, or move them to another side of the window. You can select Auto-hide to minimize them.

Calculations on models and other operations produce messages that are displayed in the Output window.You can save the information in the Output window either directly or using the clipboard. To save information directly:

1. Right-click in the window and choose Export.

   A Save As dialog box appears.
2. Enter a name for the file, select a file format (.html or .txt) and click Save.

To save information with the clipboard:

1. Select the text you want to save.
2. Right-click in the window and choose Copy.

   Alternately, you can choose Select All from the right-click menu.
3. Paste into the document of your choice.

You must use Copy – Paste to restore information from a saved file.

You can remove information from the Output window without affecting the model.

To remove messages:

1. Select the text you want to delete.
2. Do one of the following:
   - From the Right-click menu, choose Clear.
   - Press the Delete or Backspace key.

The Comments window gives you a place to add notes and comments about the model. When you save a model, comments are also saved.

Model Building Basics

As you create models, Chem3D applies standard parameters from external tables along with user-selected settings to produce the model display. There are several options for selecting your desired display settings: you can change defaults in the Model Settings dialog box, use menu or toolbar commands, or use context-sensitive menus (right-click menus) in the Model Explorer. You can also view and change model coordinates.

Internal and External Tables

Chem3D uses two types of parameter tables:

- **Internal tables**—Contain information about a specific model.

  Examples of internal tables are:
  - Measurements table
  - Z-Matrix table
  - Internal coordinates table
- **External tables**—Contain information used by all models.

  Examples of external tables are:
  - Elements, Atom Types, and Substructures tables that you use to build models.
  - Torsional Parameters tables that are used by Chem3D when you perform an MM2 computation.
  - Tables that store data gathered during Dihedral Driver conformational searches.

Standard Measurements—Standard measurements are the optimal (or equilibrium) bond lengths and angles between atoms based on their atom type. The values for each particular atom type combination are actually an average for many compounds each of which have that atom type (for example, a family of alkanes). Standard measurements allow you to build models whose 3D representation is a fair approximation of the actual geometry when other forces and interactions between atoms are not considered.

For more information on External Tables, see "Parameter Tables" on page 271.

To view an internal table:

- Choose the table from the View menu.

To view an external table:

- Point to Parameter Tables on the View menu, then choose the table to view.

> ***TIP:*** *You can superimpose multiple tables if you attach them to an edge of the GUI. One table will be visible and the others will display as selection tabs. Attached tables have the Auto-hide feature.*

To auto-hide a table:

- Push the pin in the upper right corner of the table.

  The table minimizes to a tab when you are not using it.

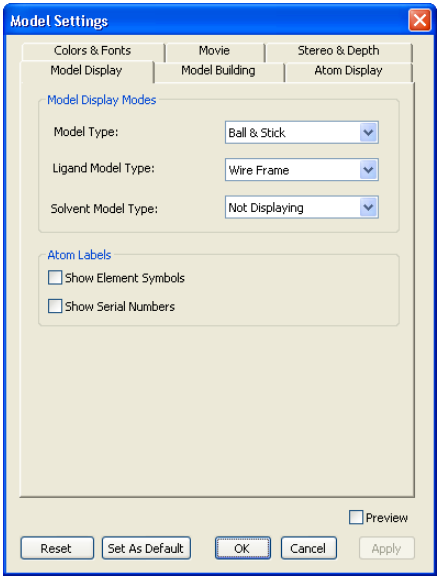
The Model Setting Dialog Box

The Chem3D Model Settings dialog box allows you to configure settings for your model.

To open the Chem3D Model Settings dialog box:

- From the File menu, choose Model Settings.

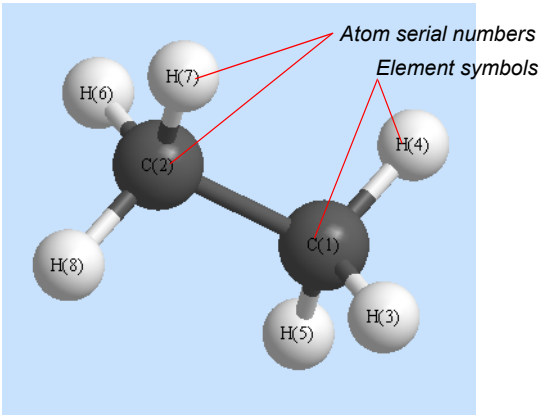
  The Settings dialog box appears:



The settings are organized into tabbed panels. To select a control panel, click one of the tabs at the top of the dialog box.

Model Display

The model of ethane shown below displays the cylindrical bonds display type (rendering type) with the element symbols and serial numbers for all atoms.



To specify the rendering type do one of the following:

- From the View menu, point to Model Display, then Display Mode, and select a rendering type.
- Activate the Model Display toolbar, click the arrow next to the Model Display icon , and select a rendering type.
- In the Model Settings dialog box, choose Model Display, and select a rendering type.

To specify the display of serial numbers and element symbols, do one of the following:

- On the View menu, point to Model Display, then click Show Serial Number or Show Atom Label.
- Activate the Model Display toolbar and click the Atom Labels and Serial Numbers icons.

- In the Model Settings dialog box, select the Atom Labels tab, and check the box next to Show Element Symbols and Show Serial Numbers.

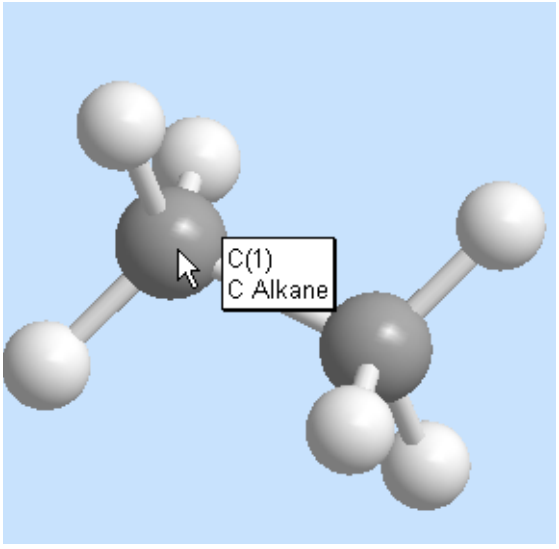
The serial number for each atom is assigned in the order of building. However, you can reserialize the atoms. For more information see "Setting Serial Numbers" on page 88.

The element symbol comes from the Elements table. The default color used for an element is also defined in the Elements table. For more information, see "Coloring by Element" on page 58 and "The Elements" on page 274.

Model Data Labels

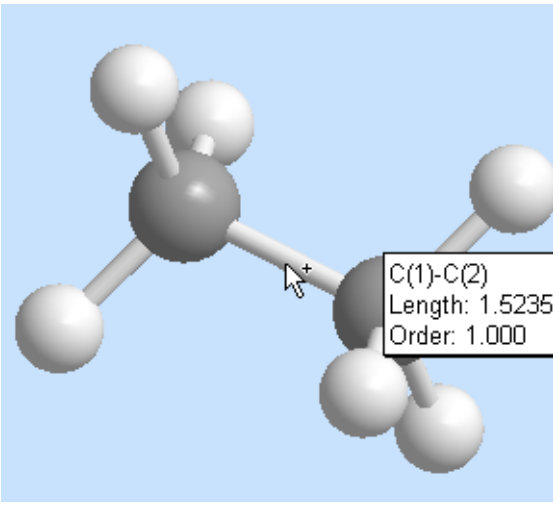
When you point to an atom, information about the atom appears in a model label pop-up window. By default, this information includes the element symbol, serial number, atom type, and formal charge.

The following illustration shows the model label for the C(1) atom of ethane.



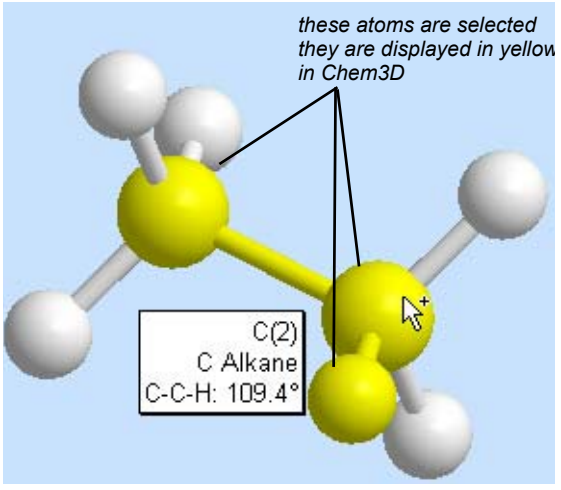
The model data changes when you point to a bond instead of an atom.

The following illustration shows the model label for the bond between C(1) and C(2).



The model data changes to reflect the atoms that are selected in the model. For example, when three contiguous atoms H(3)-C(1)-C(2) are selected, the model label includes the atom you point to and its atom type, the other atoms in the selection, and the angle.

This is shown in the following illustration.



If you select four contiguous atoms the dihedral angle appears in the model label. If you select two bonded or non-bonded atoms, the distance between those atoms appears.

To specify what information appears in atom, bond, and angle labels:

- In the Model Settings dialog box, select the Pop-up Info tab, then select the information you want to display.

Atom Types

Atom types contain much of the Chem3D chemical intelligence for building models with reasonable 3D geometries. If an atom type is assigned to an atom, you can see it in the model data when you point to it. In the previous illustration of pointing information, the selected atom has an atom type of "C Alkane".

An atom that has an atom type assigned has a defined geometry, bond orders, type of atom used to fill open valences (rectification), and standard bond length and bond angle measurements (depending on the other atoms making up the bond).

The easiest way to build models uses a dynamic assignment of atom types that occurs as you build. For example, when you change a single bond in a model of ethane to a double bond, the atom type is automatically changed from C Alkane to C Alkene. In the process, the geometry of the carbon and the number of hydrogens filling open valences changes.

You can also build models without assigning atom types. This is often quicker, but certain tasks, such as rectification or MM2 Energy Minimization, will also correct atom types because atom types are required to complete these tasks.

To assign atom types as you build:

- In the Chem3D Model Settings dialog box, select the Model Build tab, then check the Correct Atom Types checkbox.

To assign atom types after building:

- Select the atom(s) and use the Rectify command on the Structure menu.

Atom type information is stored in the Atom Types table. To view the Atom Types table:

- From the View menu, select Parameter Tables, then select atom types.xml.

Rectification

Rectification is the process of filling open valences of the atoms in your model, typically by adding hydrogen atoms.

To rectify automatically as you build, do the following:

- In the Chem3D Model Settings dialog box, select the Model Build tab, and then check the Rectify checkbox.

If you activate automatic rectification in the Model Settings dialog box, you have the option of showing or hiding hydrogens. If you turn off automatic rectification, the Show Hs and Lps command on the Model Display submenu of the View menu is deactivated, and you will not have the option of displaying hydrogens.

Bond Lengths and Bond Angles

You can apply standard measurements (bond lengths and bond angles) automatically as you build or apply them later . Standard measurements are determined using the atom types for pairs of bonded atoms or sets of three adjacent atoms, and are found in the external tables Bond Stretching Parameters.xml and Angle Bending Parameters.xml.

The Model Explorer

The Model Explorer allows users to explore the hierarchical nature of a macromolecule and alter properties at any level in the hierarchy. Display

modes and color settings are easy to control at a fine-grained level. Properties of atoms and bonds are easy to access and change.

The Model Explorer is designed as a hierarchical tree control that can be expanded/collapsed as necessary to view whatever part of the model you wish. Changes are applied in a bottom-up manner, so that changes to atoms and bonds override changes at the chain or fragment level. You can show/hide/highlight features at any level. Hidden or changed features are marked in the hierarchical tree with colored icons, so you can easily keep track of your edits. See "Working With the Model Explorer" on page 111 for more information.

Model Coordinates

Each of the atoms in your model occupies a position in space. In most modeling applications, there are two ways of representing the position of each atom: internal coordinates and Cartesian coordinates. Chem3D establishes internal and Cartesian coordinates as you build a model.

Z-matrix

Internal coordinates for a model are often referred to as a Z-matrix (although not strictly correct), and are the most commonly used coordinates for preparing a model for further computation. Changing a Z-matrix allows you to enter relations between atoms by specifying angles and lengths.

You display the Z-Matrix table by selecting it from the View menu. You can edit the values within the table, or move atoms within the model and use the Set Z-matrix submenu of the Structure menu. You can copy and paste tables to text (.txt) files or Excel spreadsheets using the commands in the context (right-click) menu.

Below is an example of the internal coordinates (Z-matrix) for ethane:

Z-Matrix

	S.N.	Atom	Bond Atom	Bond Length	Angle Atom	Angle	Dihedral Atom	Dihedral
1	1	C						
2	5	C	C(1)	1.5400				
3	6	H	C(5)	1.1220	C(1)	109.5000		
4	7	H	C(5)	1.1220	C(1)	109.5000	H(6)	109.5000
5	8	H	C(5)	1.1220	C(1)	109.5000	H(6)	109.5000
6	2	H	C(1)	1.1220	C(5)	109.5000	H(6)	60.0000
7	3	H	C(1)	1.1220	C(5)	109.5000	H(2)	109.5000
8	4	H	C(1)	1.1220	C(5)	109.5000	H(2)	109.5000

Cartesian Coordinates

Cartesian coordinates are also commonly accepted as input to other computation packages. They describe atomic position in terms of X-, Y-, and Z-coordinates relative to an arbitrary origin. Often, the origin corresponds to the first atom drawn. However, you can set the origin using commands in the Model Position submenu of the Structure menu.

Instead of editing the coordinates directly in this table, you can save the model using the Cartesian Coordinates file format (.cc1 or .cc2), and then edit that file with a text editor. You can also copy and paste the table into a text file or Excel worksheet using the commands in the context (right-click) menu.

NOTE: *If you do edit coordinates in the table, remember to turn off* Rectify *and* Apply Standard Measurements *in the* Model Build *panel of the* Model Settings *dialog while you edit so that other atoms are not affected.*

An example of the Cartesian coordinates for ethane is shown below.

Cartesian

	S.N.	Atom	X	Y	Z
1	1	C	-0.7700	0.0000	0.0003
2	2	H	-1.1445	-0.5288	0.9163
3	3	H	-1.1445	-0.5277	-0.9163
4	4	H	-1.1445	1.0576	-0.0010
5	5	C	0.7700	0.0000	0.0003
6	6	H	1.1445	-1.0576	0.0003
7	7	H	1.1445	0.5299	0.9156
8	8	H	1.1445	0.5299	-0.9150

The Measurements Table

The Measurements table displays bond lengths, bond angles, dihedral angles, and ring closures. When you first open a Measurements Table, it will be blank.

To display data in a Measurements Table:

- From the Structure menu, point to Measurements, then select the information you wish to display.

The example shows the display of Bond Lengths and Bond Angles for ethane:

Measurement

	Atoms	Actual	Optimal
1	H(8)-C(2)	1.1130	1.1130
2	H(7)-C(2)	1.1130	1.1130
3	H(6)-C(2)	1.1130	1.1130
4	H(5)-C(1)	1.1130	1.1130
5	H(4)-C(1)	1.1130	1.1130
6	C(1)-H(3)	1.1130	1.1130
7	C(2)-C(1)	1.5230	1.5230
8	H(8)-C(2)-H(7)	108.8118	109.0000
9	H(8)-C(2)-H(6)	109.0000	109.0000
10	H(8)-C(2)-C(1)	110.0000	110.0000
11	H(7)-C(2)-H(6)	109.0000	109.0000
12	H(7)-C(2)-C(1)	110.0000	110.0000
13	H(6)-C(2)-C(1)	110.0000	110.0000
14	H(5)-C(1)-H(4)	108.8118	109.0000
15	H(5)-C(1)-H(3)	109.0000	109.0000
16	H(5)-C(1)-C(2)	110.0000	110.0000
17	H(4)-C(1)-H(3)	109.0000	109.0000
18	H(4)-C(1)-C(2)	110.0000	110.0000
19	H(3)-C(1)-C(2)	110.0000	110.0000

If you edit the Actual field, you change the value in the model, and see atoms in the model move.

If you edit the Optimal value, you apply a constraint. These values are used only in Clean Up (on the Structure menu) and MM2 computations.

Deleting Measurement Table Data

You can isolate the information you in the Measurements table by deleting the records that you do not want to view. For example, you could display bond lengths, then delete everything except the carbon-carbon bonds. This would make them easier to compare.

To delete records:

- Select the records and click Delete on the right-click menu.

  Deleting records in a Measurements table does not delete the corresponding atoms.

To clear the entire table:

- On the Measurement submenu of the Structure menu, select Clear.

Chapter 2: Chem3D Tutorials

Overview

The following section gives detailed examples of some general tasks you can perform with Chem3D. For examples of MOPAC calculations, see Chapter 10, "MOPAC Computations" on page 165.

In this section:

- Tutorial 1: Working with ChemDraw on page 31.
- Tutorial 2: Building Models with the Bond Tools on page 32.
- Tutorial 3: Building Models with the Text Building Tool on page 36.
- Tutorial 4: Examining Conformations on page 39.
- Tutorial 5: Mapping Conformations with the Dihedral Driver on page 42.
- Tutorial 6: Overlaying Models on page 43.
- Tutorial 7: Docking Models on page 46.
- Tutorial 8: Viewing Molecular Surfaces on page 48.
- Tutorial 9: Mapping Properties onto Surfaces on page 49.
- Tutorial 10: Computing Partial Charges on page 52.

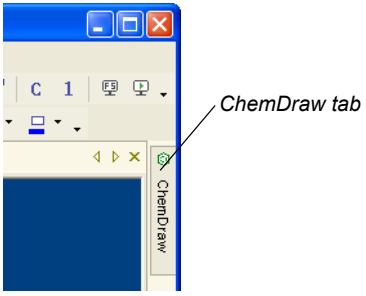
Tutorial 1: Working with ChemDraw

The following tutorial introduces model building with Chem3D. It assumes that no defaults have been changed since installation. If what you see is not like the description, you may need to reset the defaults. To reset defaults:

- From the File menu, open the Model Settings dialog box. Click the Reset button.

Open a new model window if one is not already opened. To view models as shown in this tutorial, select Cylindrical Bonds from the drop-down menu of the Model Display mode tool on the Model Display toolbar.

The installation default for the ChemDraw panel is activated, hidden. You should see a tab labeled ChemDraw on the upper right side of the GUI.



If you do not see the tab:

1. From the View menu, select ChemDraw Panel.

   The ChemDraw Panel opens in its default position, attached to the right edge of the model window.

If the tab is visible:

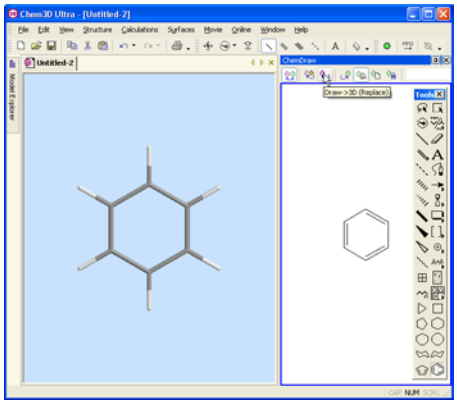
2. Click the ChemDraw tab to open the panel.

TIP: The panel default is Auto-hide. If you want the panel to stay open, push the pin on the upper right.

3. Click in the ChemDraw panel it.

   A blue line appears around the ChemDraw Panel model window, and the ChemDraw tools palette appears.
4. On the ChemDraw tools palette, select the Benzene Ring tool.
5. Click in the panel to place a benzene ring.

   The ChemDraw structure is converted into a 3D representation.

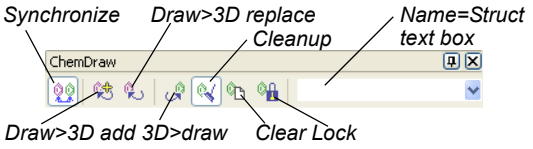


You can work with the model in Chem3D. The 2D and 3D models are hot-linked, so any change in one changes the other:

1. Double-click one of the hydrogens in the 3D model.

   A text box appears.
2. Type OH in the text box, then hit the Enter key.
3. A phenol molecule is displayed in both the Chem3D model window and the ChemDraw window.

You can turn off the hot linking by clicking the Synchronize button. If you do this, you will need to use the 3D>Draw and Draw>3D buttons to copy models between the windows.



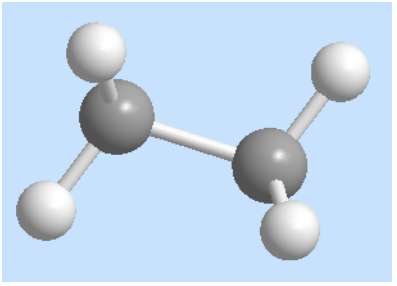
TIP: Use Ctrl+A to select the model you want to copy.

Tutorial 2: Building Models with the Bond Tools

Draw ethane using a bond tool.

1. Click the Single Bond tool .
2. Point in the model window, drag to the right and release the mouse button.

   A model of ethane appears. When you rotate the model in a later step, you will see the other hydrogen.



NOTE: If you are using default settings, hydrogens are displayed automatically.

To see the three-dimensionality of your model you can perform rotations using the Trackball tool. The Trackball Tool mimics a sphere in which your

model is centered. You can rotate your model by rotating the sphere. You have a choice of free-hand rotation, or rotating around the X, Y, or Z axis.

To perform free-hand rotation of the model with the Trackball tool:

1. Click the Trackball tool .
2. Point near the center of the model window and hold down the mouse button.
3. Drag the cursor in any direction to rotate the model.

CAUTION

Users familiar with earlier versions of Chem3D should be aware of changed behavior: the Trackball tool rotates the view only, it does not change the atoms' Cartesian coordinates.

To rotate around an axis:

1. Move the cursor to the edge of the model window.

   As you mouse over the edge of the window, the rotation bars will appear.

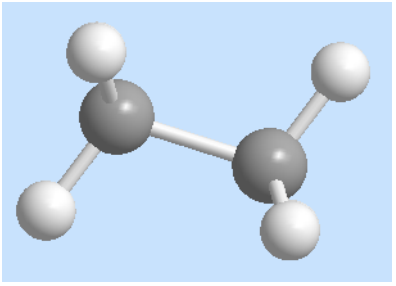
   NOTE: Rotation bars are only available when you are using the Trackball tool.

2. Drag on one of the bars to rotate the model on that axis.

   One of the bars is labeled "Rotate About Bond". You won't be able to select that one. You'll cover rotating around bonds later.

   TIP: Once you start dragging, you don't have to stay within the rotation bar's boundaries. Your model will only rotate around the chosen axis no matter where you drag your mouse.

3. Release the mouse button when the model is orientated approximately like this:

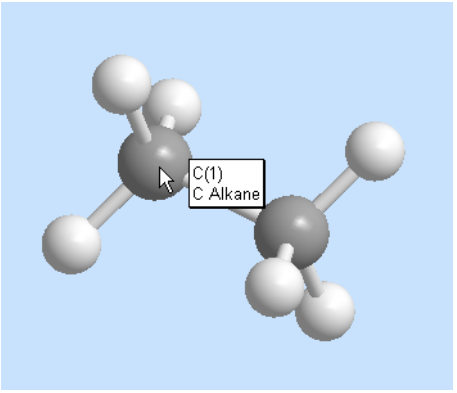


Examine the atoms and bonds in the model using the Select tool.

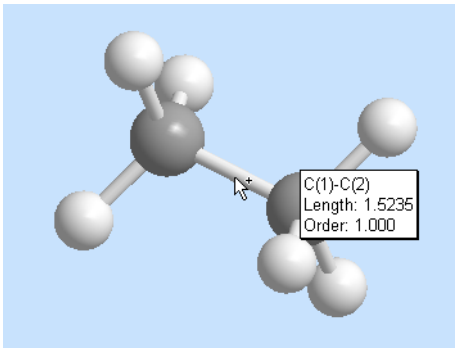
1. Click the Select tool .
2. Move the pointer over the far left carbon.

   NOTE: Depending on how much you rotated the model, the far left carbon might be C(2).

   An information box appears next to the atom you are pointing at. The first line contains the atom label. In this case, you are pointing to C(1). The second line contains the name of the atom type, C Alkane.



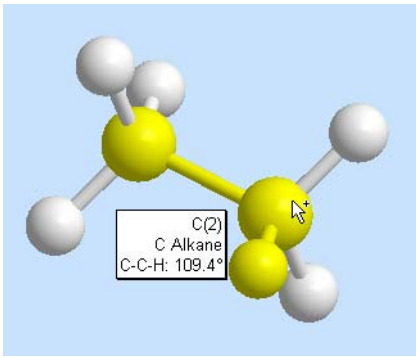
3. Move the pointer over the C-C bond to display its bond length and bond order.



To display information about angles, select several atoms.

1. Click C(1), then Shift+click C(2) and H(7).
2. Point at any of the selected atoms or bonds.

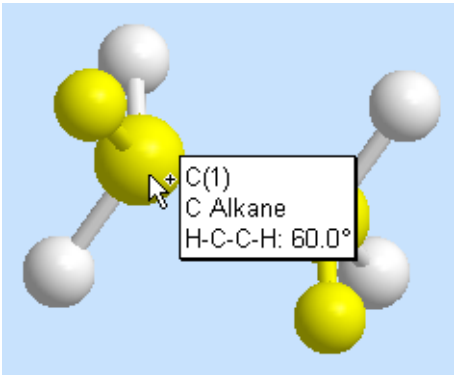
   The angle for the selection appears.



To display information about contiguous atoms:

1. Hold the Shift key and select four contiguous atoms.
2. Point at any portion of the selection.

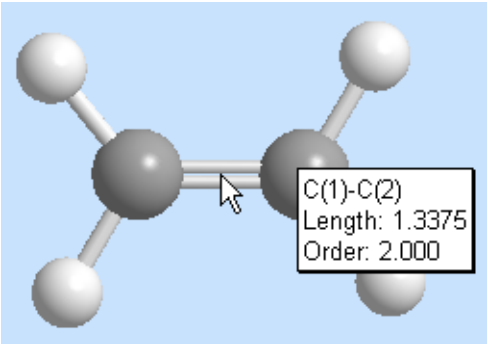
   The dihedral angle formed by those four atoms is displayed.



Change the ethane model to an ethylene model.

1. Click the Double Bond tool .
2. Drag the mouse from C(1) to C(2).
3. Point to the bond.

   The bond length decreases and the bond order increases.



Continue to build on this model to build cyclohexane.

1. Click the Select tool .
2. Click the double bond.
3. Right click, point to Bond(s), then to Order, and choose Single Bond.

   The bond order is reduced by one.

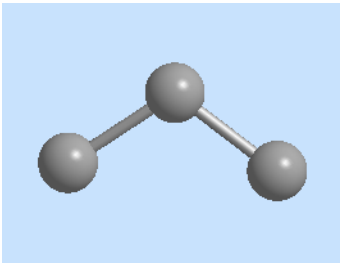
Hide the hydrogens to make it easier to build.

- On the Model Display submenu of the View menu, deselect Show Hs and Lps.

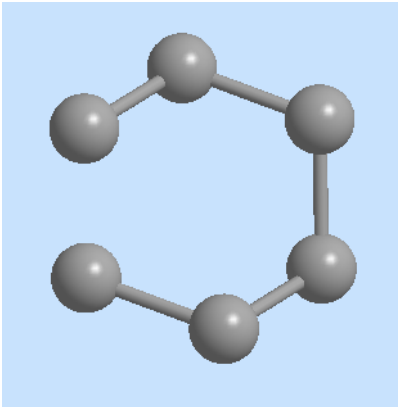
  The hydrogens are hidden.

Add more atoms to the model:

1. Click the Single Bond tool .
2. Drag upward from the left carbon.
3. Another C-C bond appears.



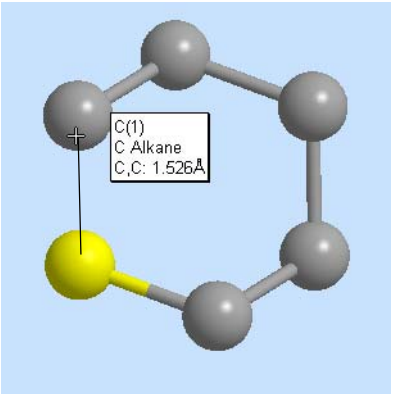
4. Continue adding bonds until you have 6 carbons as shown below.



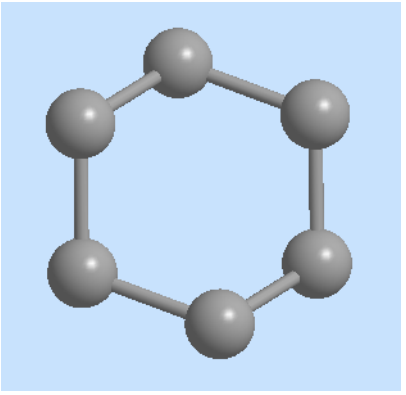
Create a ring:

1. Drag from one terminal carbon across to the other.

   The pointing information appears when you drag properly.



2. Release the mouse button to close the ring.



Add serial numbers and atom labels.

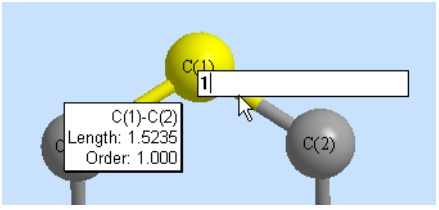
1. On the Model Display submenu of the View menu, select Show Serial Numbers, or click the Serial Number icon on the Model Display toolbar.
2. On the Model Display submenu of the View menu, select Show Atom Labels, or click the Atom Label icon on the Model Display toolbar.

NOTE: The serial numbers that appear do not reflect a normal ordering because you started with a smaller model and built up from it.

You can reserialize the atoms as follows:

1. Select the Text Building tool .
2. Click the first atom.

   A text box appears on the atom.



3. Type the number you want to assign to this atom (1 for this example).
4. Press the Enter key.

   The first atom is renumbered as (1).
5. Double-click each of the atoms in the order you want them to be numbered.

   Each time you double-click an atom to serialize it, the new serial number is one greater than the serial number of the previously serialized atom.
6. From the Model Display submenu of the View menu, choose Show Hs and Lps and examine the model using the Trackball Tool .

   The hydrogens appear as far apart as possible.

Because you built the structure by using bond tools, you may have distorted bond angles and bond lengths.

To correct for distorted angles and lengths:

1. From the Edit menu, choose Select All.

   All of the atoms in the model are selected.
2. From the Structure menu, choose Clean Up Structure.

To locate an energy minimum for your structure which represents a stable conformation of your model, click the MM2 Minimize Energy tool MM2 on the Calculation toolbar.

For more information about MM2 and energy minimization see MM2 on page 136.

After the minimization is complete:

1. From the File menu, choose Save.
2. Select a directory in which to save the file.
3. Type tut1 in the text box at the bottom of the dialog box.
4. Click Save.
5. Click the model window to activate it.
6. From the File menu, choose Close Window.

Tutorial 3: Building Models with the Text Building Tool

This tutorial illustrates alternative methods to build models using the Text Building Tool. You will start by opening the file you saved in the first tutorial:

1. From the File menu, choose Open.
2. Locate and select the file, tut1, that you created in the previous tutorial.
3. Click Open.

Replacing Atoms

To change one element into another:

1. Click the Text Building tool .
2. Click a hydrogen atom attached to C(1).

   A text box appears.
3. Type C.

   NOTE: Element symbols and substructure names are case sensitive. You must type an uppercase C to create a carbon atom.
4. Press the Enter key.

   The hydrogen attached to C(1) is changed to a carbon. The valence is filled with hydrogens to form a methyl group because Automatic Rectification is turned on.

You don't have to select the Text tool in order to use it. Double-clicking with any other tool selected has the same effect as single-clicking with the Text tool. To demonstrate this, let's replace two more hydrogens using an alternative method:

1. Select the Trackball tool so that you can rotate your model to get a better view of what you are building.
2. Double-click two more hydrogens to change them to methyl groups.

TIP: Notice that the "C" you entered previously in the Text tool remains as the default until you change it. You only have to double-click, and press the Enter *key.*

Now, refine the structure to an energy minimum to take into account the additional interactions imposed by the methyl groups by clicking the MM2 tool on the Calculation toolbar.

When the minimization is complete:

1. From the File menu, choose Save As.
2. Type tut2a.
3. Select a directory in which to save the file.
4. Click Save.

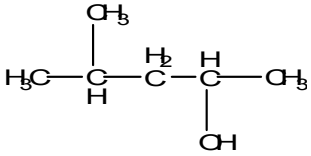
Save a copy of the model using a different name:

1. From the File menu, choose Save As.
2. Type tut2b.
3. Select a directory in which to save the file.
4. Click Save.

We'll be using these two copies of your model in later tutorials.

Using Labels to Create Models

You can also create models by typing atom labels (element symbols and numbers) into a text box.



To build the model of 4-methyl-2-pentanol shown above:

1. From the File menu, choose New, or click the new file tool on the Standard toolbar.
2. Click the Text Building tool .
3. Click in the empty space in the model window.

   A text box appears where you clicked.
4. In the text box, type CH3CH(CH3)CH2CH(OH)CH3.

   You type labels as if you were naming the structure: pick the longest chain of carbons as the backbone, and specify other groups as substituents. Enclose substituents in parentheses after the atom to which they are attached.

5. Press the Enter key.

TIP: The Text building tool will also accept structures in SMILES notation, either typed in or cut and pasted from other documents.

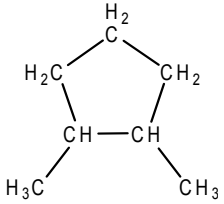
Another, simpler, way of building this model is to type Pentane in the Name=Struct text box and then modify the appropriate hydrogens.

Refine the model as follows.

1. Click the Select tool
2. Select the model by dragging diagonally across it.
3. From the Structure menu, choose Clean Up.

If you want a more accurate representation of a low energy conformation, optimize the geometry of the model by clicking the MM2 tool on the Calculation toolbar.

To specify text equivalent to the structure of 1,2-dimethyl cyclopentane shown below:



1. From the File menu, choose New.
2. Click the Text Building tool .
3. Click in the empty space in the model window.
4. Type CH(CH3)CH(CH3)CH2CH2CH2.
5. Press the Enter key.

   The *trans*-isomer appears.

6. Select the model and choose Clean Up from the Structure menu.

TIP: You don't have to click the Select tool every time you want to select something. Just hold down the letter S on your keyboard while working with any building tool, and you temporarily activate the Select tool.

You cannot specify stereochemistry when you build models with labels. The structure of 1,2-dimethyl cyclopentane appears in the trans conformation.

To obtain the *cis*-isomer:

1. Click the Select tool .
2. Select C(1).
3. From the Structure menu, choose Invert.

   The *cis*-isomer appears. You can rotate the molecule to see the differences between the isomers after you invert the molecule.

Using Substructures

Labels are useful to build simple structures. However, if you make larger, more complex structures, you will find it easier to use a combination of labels and pre-defined substructures.

Over 200 substructures are pre-defined in Chem3D. These substructures include the most commonly used organic structures.

TIP: Pre-defined substructures are listed in the substructures.xml file. You can view the list by pointing to Parameter Tables on the View menu and selecting Substructures. Text typed in the text box is case sensitive. You must type it exactly as it appears in the Substructures table.

Build a model of nitrobenzene:

1. From the File menu, choose New.
2. Click the Text Building tool .
3. Click the empty space in the model window.

4. Type Ph(NO2) in the text box.
5. Press the Enter key.

   A model of nitrobenzene appears.

The substructure in this example is the phenyl group. Substructures are defined with specific attachment points for other substituents. For phenyl, the attachment point is C(1).

Build a peptide model:

1. From the File menu, choose New.
2. Click the Text Building tool A.
3. Click an empty space in the Model window.

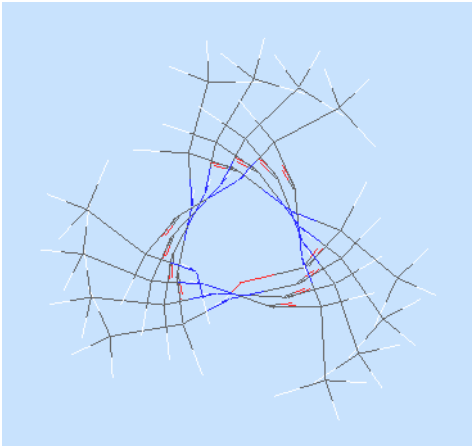
   A text box appears.
4. Type H(Ala)12OH.
5. Press the Enter key.
6. Rotate this structure to see the alpha helix that forms.

Change the model display type:

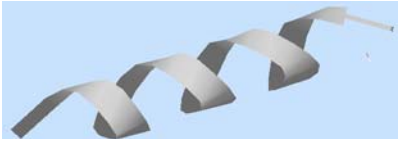
1. Click the arrow on the right side of the Model Display Mode tool on the Model Display toolbar.
2. Select Wire Frame as the Model Type.

TIP: You can also click on the icon. Successive clicks cycle through the Display Mode options.

3. Select the Trackball tool, and rotate the model so you are viewing it down the center of the helix as shown below:



4. Use the Model Display Mode tool to choose Ribbons as the Model Type to see an alternative display commonly used for proteins.



Tutorial 4: Examining Conformations

This tutorial uses steric energy values to compare two conformations of ethane. The conformation with the lower steric energy value represents the more likely conformation.

Build ethane:

1. Draw a single bond in the ChemDraw panel.

   A model of ethane appears.
2. View the Measurements table:
   a. From the Structure menu, point to Measurements, and then choose Bond Lengths.

b. From the Structure menu, point to Measurement, and then choose Bond Angles.

NOTE: If the Measurements table appears along side the Model Explorer, you can stack the windows by locking the Model Explorer window open and dragging the Measurements table on top of it.

The information you chose appears in the Measurements table. The measurements in the Actual and Optimal columns are nearly identical. The Actual column represents the measurements for the model in the active window. The Optimal measurements (for bond lengths and bond angles only) represent the standard measurements in the Bond Stretching and Angle Bending parameter tables.

Measurement

	Atoms	Actual	Optimal
1	H(8)-C(2)	1.1130	1.1130
2	H(7)-C(2)	1.1130	1.1130
3	H(6)-C(2)	1.1130	1.1130
4	H(5)-C(1)	1.1130	1.1130
5	H(4)-C(1)	1.1130	1.1130
6	H(3)-C(1)	1.1130	1.1130
7	C(1)-C(2)	1.5230	1.5230
8	H(8)-C(2)-H(7)	108.8118	109.0000
9	H(8)-C(2)-H(6)	109.0000	109.0000
10	H(8)-C(2)-C(1)	110.0000	110.0000
11	H(7)-C(2)-H(6)	109.0000	109.0000
12	H(7)-C(2)-C(1)	110.0000	110.0000
13	H(6)-C(2)-C(1)	110.0000	110.0000
14	H(5)-C(1)-H(4)	108.8118	109.0000
15	H(5)-C(1)-H(3)	109.0000	109.0000
16	H(5)-C(1)-C(2)	110.0000	110.0000
17	H(4)-C(1)-H(3)	109.0000	109.0000
18	H(4)-C(1)-C(2)	110.0000	110.0000
19	H(3)-C(1)-C(2)	110.0000	110.0000

XYZ Cartesian | Z-Matrix | Measure...

Chem3D shows the most common conformation of a molecule. You can rotate parts of a molecule, such as a methyl group, to see other conformations. Rotate the orientation of the model to obtain a Newman projection (viewing the model along a bond.) This orientation helps clarify the conformations of ethane.

To rotate a methyl group on an ethane model:

1. Click the Trackball tool .

   When you mouse over the edges of the model window, the Rotation Bars appear.

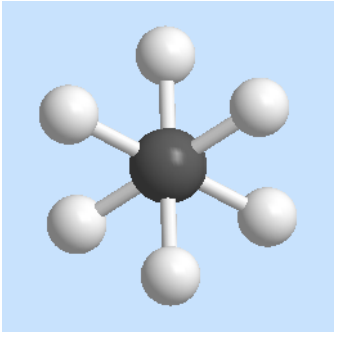
   Only the X- and Y-rotation bars are active. These Rotations bars are always active because they are not dependent on any atoms being selected.

2. Click the X-Axis rotation bar and drag to the right.

   As you drag, the status bar shows details about the rotation.

3. Stop dragging when you have an end-on view of ethane.

   This staggered conformation, where the hydrogens on adjoining carbons are a maximum distance from one another (which represents the global minimum on a potential energy plot) represents the most stable conformation of ethane.



To examine this result numerically, calculate the steric energy of this conformation and then compare it to a higher energy (eclipsed) conformation.

1. From the Calculations menu, point to MM2, then choose Compute Properties.

   The Compute Properties dialog box appears. The Properties tab should show Pi Bond Orders and Steric Energy Summary selected as the default. If it does not, select them.

   TIP: Use Shift-click to select multiple properties.

2. Click Run.

   The Output box appears beneath the model window, with Steric Energy results displayed. The last line displays the total energy.

NOTE: The values of the energy terms shown are approximate and may vary slightly based on the type of processor used to calculate them.

To obtain the eclipsed conformation of ethane, rotate a dihedral angle (torsional angle). Rotating a dihedral angle is a common way of analyzing the conformational space for a model.

To view dihedral angles:

1. From the Structure menu, point to Measurement, and then choose Dihedral Angles.

   All of the model's dihedral angles are added to the bottom of the Measurements table.

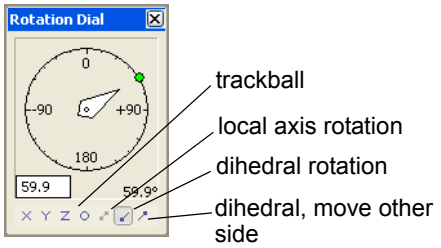
2. Click the H(3)-C(1)C(2)-H(8) dihedral record to select the corresponding atoms in the model.

   NOTE: Although the serial numbers and element symbols are shown in the Measurements table, they do not appear in your model.

To help keep visual track of the atoms as you change the dihedral angle you can display the serial numbers and element symbols for the selected atoms.

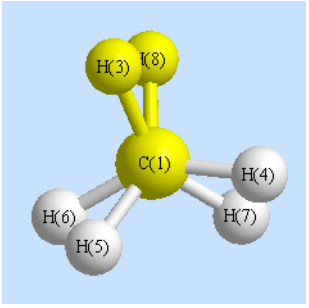
- From the Model Display submenu of the View menu, select Show Serial Numbers and Show Element Symbols.

1. Click the arrow next to the Trackball tool, and tear off the rotation dial by dragging on the blue bar at the top.

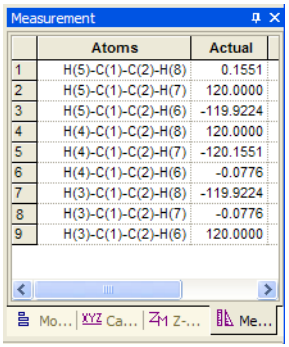


   The Rotation dial should show the angle of the selected dihedral, approximately 60°, and dihedral rotation should be selected.

2. Grab the green indicator button, and rotate the dial to 0.0.



In the Measurements table, notice that the dihedral for H(3)-C(1)-C(2)-H(8) is now minus 0 degrees, as shown in the model.



To compute steric energy:

1. From the Calculations menu, point to MM2, then choose Compute Properties.

   NOTE: The property tab defaults should remain as in the previous calculation.

2. Click Run.

The final line in the Output box appears as follows:

```
  1,4 VDW:          1.7726
Total:              3.9061
The steric energy for frame    1: 3.906 kcal/mole
Calculation completed
```

NOTE: The values of the energy terms can vary slightly based on the type of processor used to calculate them.

The steric energy for the eclipsed conformation (~3.9 kcal/mole) is greater in energy than that of the staggered conformation (~1 kcal/mole), indicating that the staggered configuration is the conformation that is more likely to exist.

NOTE: As a rule, steric energy values should only be used for comparing different conformations of the same model.

Tutorial 5: Mapping Conformations with the Dihedral Driver

The dihedral driver allows you to map the conformational space of a model by varying one or two dihedral angles. At each dihedral angle value, the model is energy minimized using the MM2 force field and the steric energy of the model is computed and graphed. After the computation is complete you can view the data to locate the models with the lowest steric energy values and use these as starting points for further refinement in locating a stationery point.

To use the dihedral driver:

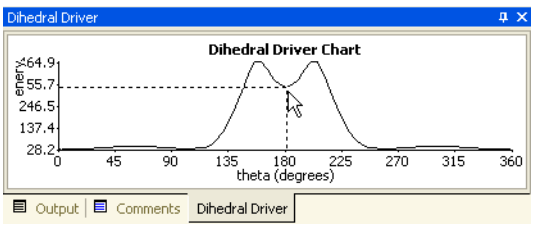
1. Select the bond in your model that defines the dihedral angle of interest.
2. Choose Dihedral Driver from the Calculations menu.

   The Dihedral Driver window opens. When the computation is completed, a graph is displayed showing the energy (kcal) vs. theta (angle of rotation).

To view the conformation at any given point:

1. Point to a location (specific degree or energy setting) inside the Dihedral Driver Window.

   A dashed-line box appears. As you move the mouse, the box moves to define a specific point on the graph.



2. Click on the point of interest.

The model display rotates the dihedral to the selected conformation.

NOTE: The dihedral is rotated in 5 degree increments through 360 degrees for a total of 72 conformations to produce the graph. You can view the minimized energy values for each point in the Output window.

To rotate the other dihedral angle (other end of the bond):

- Right-click in the Dihedral Driver window and choose Exchange.

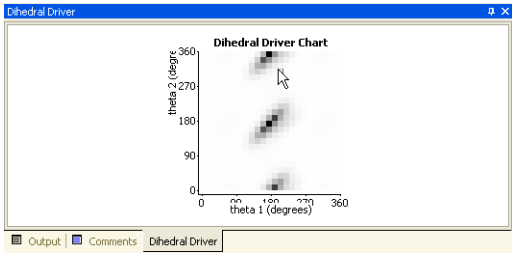
Rotating two dihedrals

To rotate two dihedrals:

1. Use Shift+click to select two adjacent bonds.

   In this case, the middle atom's position remains fixed
2. Choose Dihedral Driver from the Calculations menu.

   The Dihedral Driver window opens. When the computation is completed, a graph is displayed showing theta 1 vs. theta 2.



NOTE: The graph is the result of rotating one angle through 360° in 15° increments while holding the other constant. The second angle is then advanced 15° and the operation is repeated.

To view the conformation at any given point:

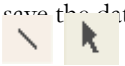
- Click any block in the graph.

The model display rotates both dihedrals to the selected conformation.

Customizing the Graph

You can use the right-click menu to set the rotation interval used for the computation. You can also select display colors for the graph, background, coordinates, and labels.

You also use the right-click menu to copy the graph, or it's data set, to other applications, or to save the data.



Tutorial 6: Overlaying Models

Overlays are used to compare structural similarities between models, or conformations of the same model. Chem3D provides two overlay techniques:

- a "Fast Overlay" algorithm
- the traditional "do it by hand" method based on minimization calculations

This tutorial describes the Fast Overlay method. For the Minimization Method, see Comparing Models by Overlay on page 109. The Minimization Method is more accurate, but the Fast Overlay algorithm is more robust. In both tutorial examples, you will superimpose a molecule of Methamphetamine on a molecule of Epinephrine (Adrenalin) to demonstrate their structural similarities.

1. From the File menu, choose New Model. Open the Model Explorer if it is not already open.
2. Choose the Text tool from the Building Toolbar and click in the model window.

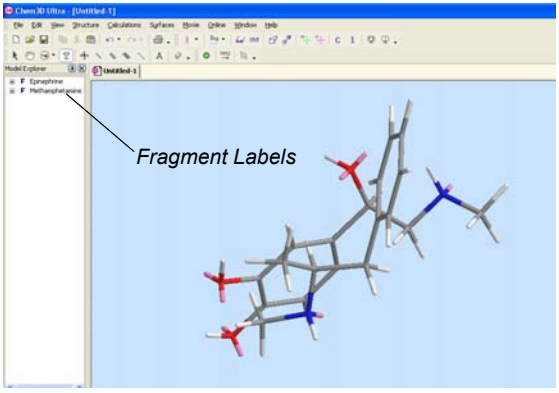
   A text box appears.
3. Type Epinephrine and press the Enter key.

A molecule of Epinephrine appears.

TIP: If you leave out the upper case "E", Chem3D will display an "Invalid Label" error message.

4. Click in the model window again to open another text box.
5. Select the entire word Epinephrine, replace it with Methamphetamine, and press the Enter key.

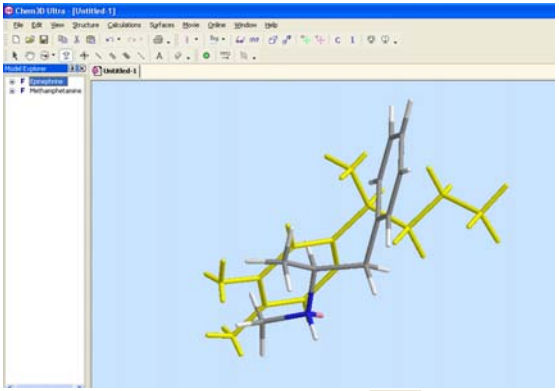
   The list of atoms in the Model Explorer is replaced with two Fragment objects, labeled Epinephrine and Methamphetamine.



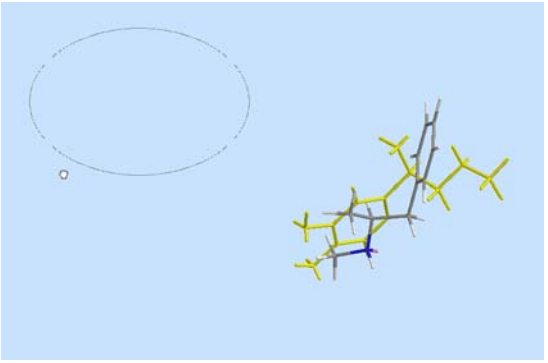
The two fragments are hopelessly jumbled together at this point, so you might want to separate them before you proceed.

1. Click one of the fragment names in the Model Explorer.

   The entire fragment is selected.

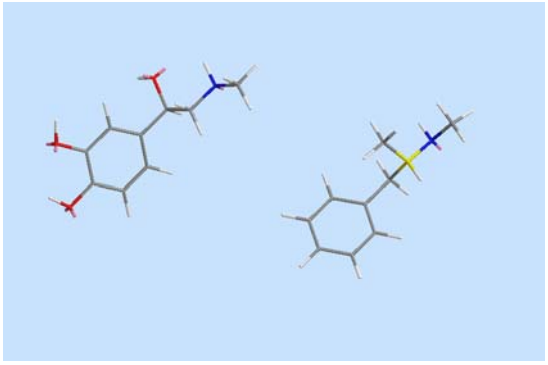


2. Click the Move Objects tool.
3. Drag the selected fragment away from the other fragment.



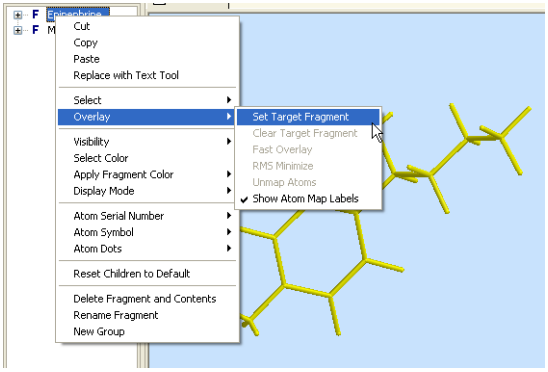
A box or oval indicates the position of the fragment while you are moving it.

TIP: You can rotate a fragment separately from the whole model by selecting at least one atom in it and using the Shift key with the trackball tool. Try this to re-orient the fragments as in the illustration below.

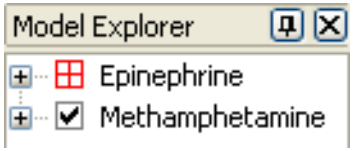


At this point, you have to decide which of the fragments will be the target. In this simple example, with only two compounds, it doesn't really matter. You might, however, have cases where you want to overlay a number of compounds on a specific target. Chem3D allows multiple overlays. The Model Explorer makes it easy to hide compounds you are not actively working with, and to display any combination of compounds you want.

1. Click the Epinephrine fragment to select it.
2. Point to Overlay on the context (right-click) menu, and click Set Target Fragment.



The icon on the fragment changes to a target.



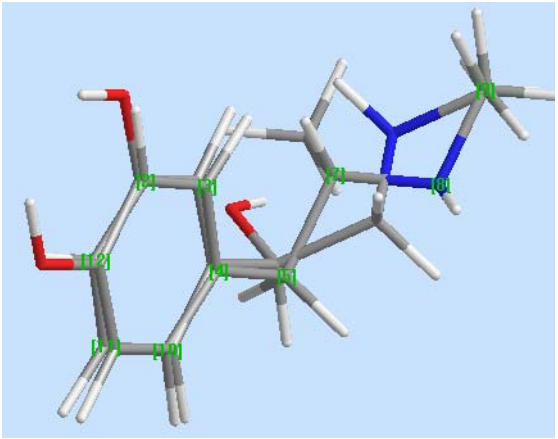
3. Select the Methamphetamine fragment.

TIP: The check in the box next to Methamphetamine does not mean that it is selected, it means that it is visible. (Try it. This is how you work with multiple overlays.) You must click on the fragment name for the Fast Overlay command to become active.

4. Choose Fast Overlay from the Overlay submenu on the context menu.

   The fragments are overlaid. The numbers show the serial numbers of the target atoms that the matching overlay atoms correspond to.

TIP: You can designate a group, rather than the entire fragment, as the target. In some cases, this will give more useful results.



To turn off the Fast Overlay mode:

- Choose Clear Target Fragment from the Overlay submenu.

Tutorial 7: Docking Models

The Dock command enables you to position a fragment into a desired orientation and proximity relative to a second fragment. Each fragment remains rigid during the docking computation.

The Dock command is available when two or more distances between atoms in one fragment and atoms in a second fragment are specified. These distances are entered into the Optimal field in the Measurements table.

You can use docking to simulate the association of regions of similar lipophilicity and hydrophilicity on two proximate polymer chains. There are four steps:

A. Build a polymer chain:

1. Open a new Model window and select the Text Building tool.
2. Click in the model window.

   A text box appears.
3. Type (AA-mon)3(C2F4)4(AA-mon)3H in the text box.
4. Press the Enter key.

   A polyacrylic acid/polytetrafluoroethylene block copolymer appears in the model window. The text, (AA-mon)3, is converted to a polymer segment with three repeat units of acrylic acid. The text, (C2F4)4, is converted to a polymer segment with four repeat units of tetrafluoroethylene.

B. Build a copy of the chain:

Double-click in the model window well above and to the right of the first polyacrylic acid/polytetrafluoroethylene block copolymer molecule.

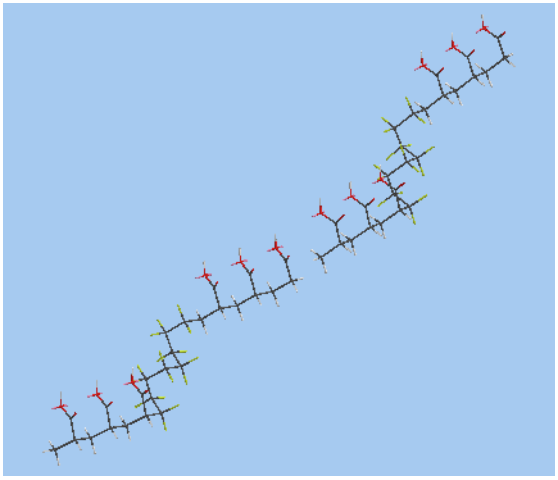
A second polymer molecule appears above the first polyacrylic acid/polytetrafluoroethylene block copolymer molecule.

C. Orient the chains:

1. Click in the empty space in the model window to deselect any atoms in the model window.
2. Click the arrow on the Trackball tool to open the Rotation Dial tool.
3. Select the Y axis, and drag the dial to show 55°.

TIP: To get exactly 55° you will probably have to edit the value in the number box. After editing, you must press the Enter key. The value displayed in the right corner of the dial should be the same as in the number box.

The resulting model appears as shown in the following illustration (the second model may appear in a different position on your computer):



D. set optimal distances between atoms in the two fragments:

The Optimal distance determines how closely the molecules dock. In this tutorial, you will set the distance to 5Å.

1. In the Model Explorer, select C(6) in Fragment 1.

   Hint: It's in the AA-mon 2 group.

2. Locate the C(98) atom in Fragment 2 (AA-mon 12 group) and Ctrl-click to select it also.
3. In the Structure menu, point to Measurements and choose Set Distance Measurement.

   The Measurements table opens, (if it is already open as a tabbed window, it becomes active) displaying the C(98)-C(6) pair.
4. Click the Optimal cell.
5. Type 5 and press the Enter key.

   The optimal distance between C(6) and C(98) is specified as 5.000Å.

To have a reasonable dock, you must specify *at least four atom pairs*. Repeat steps 1 through 5 for matching atom pairs throughout the fragments. For example, if you choose one pair from each group your list might look like the following:

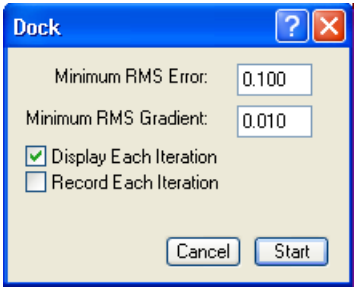
Atoms	Actual	Optimal
C(1)-C(93)	21.2034	5.0000
C(98)-C(6)	21.1840	5.0000
C(104)-C(12)	21.2863	5.0000
C(108)-C(16)	21.1957	5.0000
C(22)-C(114)	20.6472	5.0000
C(28)-C(120)	20.7001	5.0000
C(34)-C(126)	20.1410	5.0000
C(133)-C(41)	20.3559	5.0000
C(45)-C(137)	20.3218	5.0000
C(50)-C(142)	20.4350	5.0000

Ignore the distances in the Actual cell because they depend on how the second polymer was positioned relative to the first polymer when the second polymer was created.

To begin the docking computation:

1. From the Structure menu, choose Dock.

   The Dock dialog box appears.

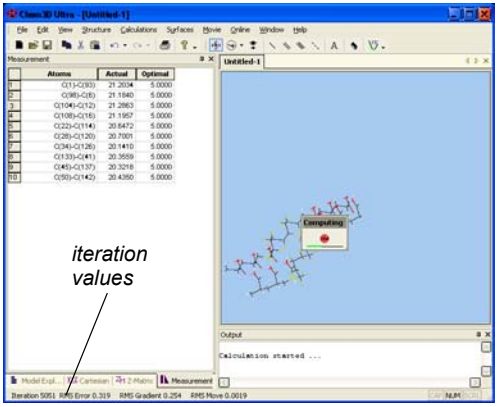


2. Type 0.100 for the Minimum RMS Error value and 0.010 for the Minimum RMS Gradient.

   The docking computation stops when the RMS Error or the RMS Gradient becomes less than the Minimum RMS Error and Minimum RMS Gradient value.
3. Click Display Every Iteration.

   This allow you to see how much the fragments have moved after each iteration of the docking computation.

To save the iterations as a movie, click Record Each Iteration.

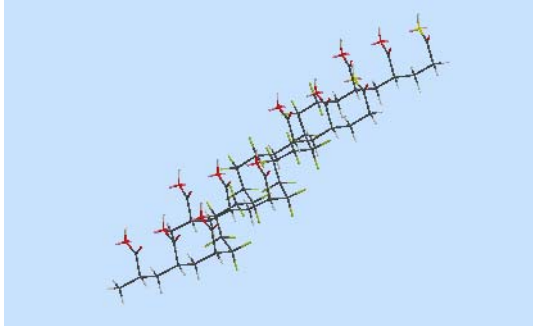


Note that while the docking computation proceeds, one molecule remains stationary and the second molecule moves.

To stop the docking computation before it reaches it's preset RMS values, click Stop Calculation on the Calculation toolbar. Both docking and recording are stopped.

The Status bar displays the values describing each iteration of the docking computation.

The following illustration shows the docked polymer molecules.



The following illustration shows the distances between atom pairs at the completion of the docking computation. The distances in the Actual cell are close to the distances in the Optimal cell.

Measurement

	Atoms	Actual	Optimal
1	C(1)-C(93)	5.0822	5.0000
2	C(6)-C(98)	5.1445	5.0000
3	C(12)-C(104)	5.0399	5.0000
4	C(16)-C(108)	5.0804	5.0000
5	C(114)-C(22)	4.9278	5.0000
6	C(120)-C(28)	4.9188	5.0000
7	C(34)-C(126)	5.0133	5.0000
8	C(41)-C(133)	4.9953	5.0000
9	C(137)-C(45)	5.0634	5.0000
10	C(142)-C(50)	5.1013	5.0000

Your results may not exactly match those described here. The relative position of the two fragments or molecules at the start of the docking computation can affect your results. For more accurate results, lower the minimum RMS gradient.

Tutorial 8: Viewing Molecular Surfaces

Frontier molecular orbital theory says that the highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) are the most important MOs affecting a molecule's reactivity. This tutorial examines the reactivity of double bonds by looking at the simplest molecule containing a double bond, ethene.

Create an ethene model:

1. From the File menu, choose New.
2. Draw a double bond in the ChemDraw panel.

   A molecule of ethene appears.

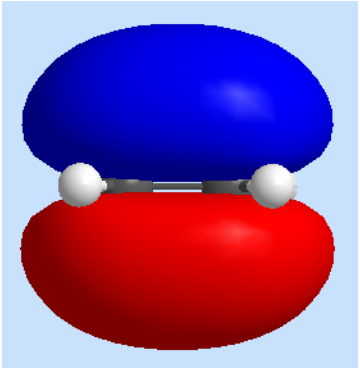
Before you can view the molecular orbital surface, you must calculate it.

3. From the Calculations menu, point to Extended Huckel and select Calculate Surfaces.

To view the Highest Occupied Molecular Orbital (HOMO):

4. From the Surfaces menu, point to Choose Surface, and select Molecular Orbital.
5. From the Surfaces menu, point to Molecular Orbital to see the HOMO/LUMO options. Select HOMO (N=6).

   The pi bonding orbital surface appears.

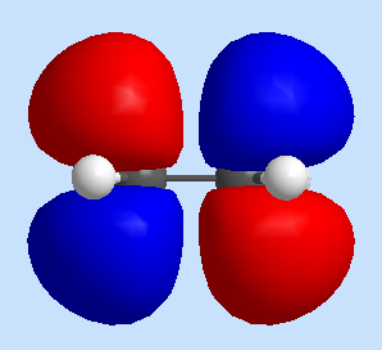


NOTE: You may need to rotate the molecule to view the orbitals.

To view the Lowest Unoccupied Molecular Orbital (LUMO):

1. From the Surfaces menu, point to Molecular Orbital to see the HOMO/LUMO options. Select LUMO (N=7).

   The pi antibonding orbital surface appears.

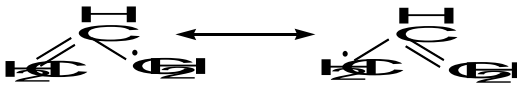


These are only two of twelve different orbitals available. The other ten orbitals represent various interactions of sigma orbitals. Only the pi orbitals are involved in the HOMO and the LUMO. Because the HOMO and LUMO control the reactivity of a molecule, you can conclude that it is the pi bonding interactions of ethene that control its reactivity. This is a specific case of a more general rule: pi bonds are more reactive than sigma bonds.

Tutorial 9: Mapping Properties onto Surfaces [ULTRA]

NOTE: This example is designed to demonstrate Gaussian minimization. You can also do it using CS MOPAC or Extended Hückel calculations.

The allyl radical, $CH_2=CHCH_2\cdot$, is a textbook example of resonance-enhanced stabilization:



To examine Radicals with Spin Density surfaces:

1. From the File menu, choose New.
2. Type 1-propene in the ChemDraw Name=Struct text box.

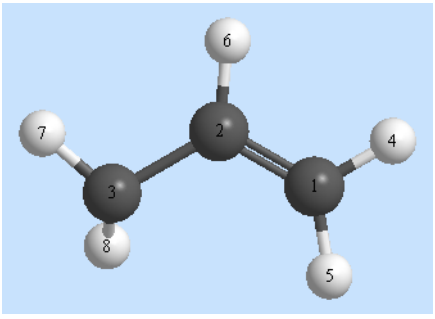
   A molecule of 1-propene appears.

Create a radical:

1. Select the H9 hydrogen.
2. Press Delete.

   A dialog box appears asking if you want to turn off rectification. Chem3D is chemically intelligent, and knows that in most cases carbon atoms have four substituents. Radicals are one of the rare exceptions.
3. Click Turn Off Automatic Rectification.

   The propene radical is displayed.



4. From the Calculations menu, point to Gaussian, and choose Minimize Energy.
5. In the Theory tab, set the Method to PM3, and the Wave Function to Open Shell (Unrestricted).
6. Also in the Theory tab, set the Spin Multiplicity to 2.

NOTE: If you are doing this tutorial with CSMOPAC, there is no Spin Multiplicity setting.

This molecule is intended to be a radical, and setting the Spin Multiplicity ensures that it is.

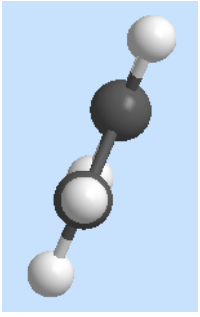
One of the best ways to view spin density is by mapping it onto the Total Charge Density surface. This allows you to see what portions of the total charge are contributed by unpaired electrons, or radicals.

To view Spin Density mapped onto Total Charge Density Surface:

1. In the Properties tab, select Molecular Surfaces and Spin Density (use Shift-click).
2. Press Run.

   The calculation toolbar appears.

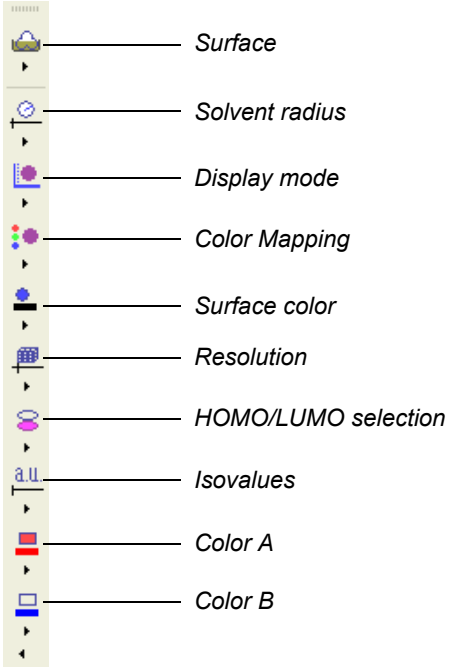
When the calculation is finished, select the Trackball tool and rotate the model back and forth. It should be completely planar.



To complete this tutorial, you will need to adjust a number of surface settings. For convenience, activate the Surfaces toolbar.

1. From the View menu, point to Toolbars, and choose Surfaces.

   The Surfaces toolbar appears. Drag it into the workspace for added convenience.

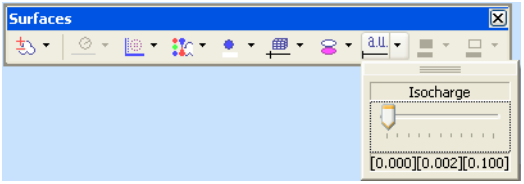


2. On the Surfaces toolbar, point to Surface and select Total Charge Density.

   The icon changes to denote the surface selected.

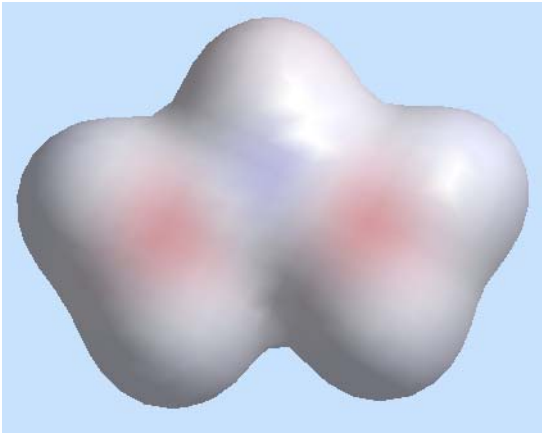
3. On the Surfaces toolbar, point to Display Mode and choose Translucent.
4. On the Surfaces toolbar, point to Color Mapping and choose Spin Density.
5. On the Surfaces toolbar, choose Isocharge.

   The Isocharge tool appears.



6. Set the isocharge to 0.0050. (The number in the middle is the current setting.)

NOTE: Isovalues are used to generate the surface. You can adjust this value to get the display you want. The illustration below was made with the setting of 0.0050.



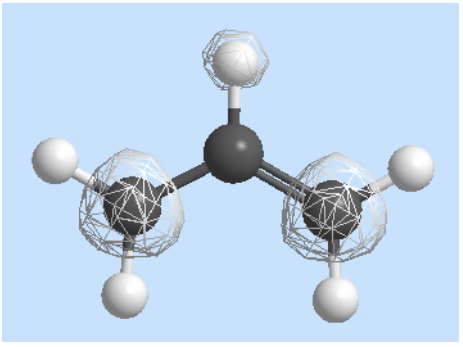
Most of the surface is grey, indicating that there is no contribution to it from unpaired electrons. The areas of red centered over each of the terminal carbons is a visual representation of the expected delocalization of the radical—there is some radical character simultaneously on both of these carbons.

Now, hide this surface:

- Click the Surfaces icon to toggle the surface off.

Determine the raw spin density alone, not mapped onto the charge density surface.

1. On the Surfaces toolbar, point to Surface, and select Total Spin Density.
2. From the Surfaces menu, point to Surfaces, and choose Wire Mesh.
3. Set Isospin to 0.001.



There is a large concentration of unpaired spin over each of the terminal carbons and a small concentration over the central hydrogen. This extra little bit of spin density is not very significant—you could not even see it when looking at the mapped display earlier, but the calculations show that it is, in fact, there.

Tutorial 10: Computing Partial Charges

To compute the charge of a molecule, the number of electrons contributed by each of its atoms can be subtracted from the number of protons in the nucleus of each of its atoms. Each atom of a molecule contributes an integral charge to the molecule as a whole. This integral contribution is known as the formal charge of each atom.

Certain types of atoms in Chem3D deal with this explicitly by having non-integral formal charges. For example, the two oxygen atoms in nitro-benzene each have charges of -0.500 because there is one electron that is shared across the two N-O bonds.

However, as shown above, electrons in molecules actually occupy areas of the molecule that are not associated with individual atoms and can also be attracted to different atomic nucleii as they move across different atomic orbitals. In fact, bonds are a representation of the movement of these electrons between different atomic nucleii.

Because electrons do not occupy the orbitals of a single atom in a molecule, the actual charge of each atom is not integral, but is based on the average number of electrons in the model that are occupying the valence shells of that atom at any given instant. By subtracting this average from the number of protons in the molecule, the partial charge of each atom is determined.

Visualizing the partial charge of the atoms in a molecule is another way to understand the model's reactivity. Typically the greater the partial charge on an atom, the more likely it is to form bonds with other atoms whose partial charge is the opposite sign.

Using the theories in Extended Hückel, MOPAC, or Gaussian, you can compute the partial charges for each atom. In the following example, the partial charges for phenol are computed by Extended Hückel.

1. From the File menu, choose New.

   Click the Text Building tool , click in the model window, type PhOH in the text box, and press the Enter key.

   A molecule of phenol is created.

To compute Extended Hückel charges:

- From the Calculations menu, point to Extended Hückel and choose Calculate Charges.

  Messages are added to the Output box, listing the partial charge of each atom.

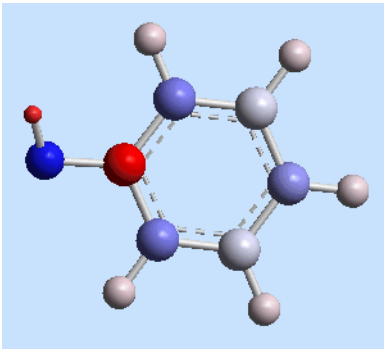
You can graphically display partial charges in the following ways:

- By coloring atoms.
- By varying the size of atom spheres.
- By varying the size of the dot surfaces.

To display partial charges:

1. From the File menu, choose Model Settings.
2. Click the Model Display tab.
3. Select the Color by Partial Charge radio button.

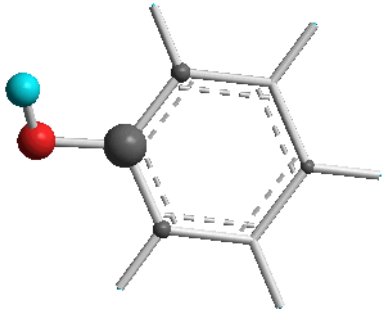
   All of the atoms are colored according to a scale from blue to white to red. Atoms with a large negative partial charge are deep blue. Atoms with a large positive partial charge are deep red. As the magnitude of the charges approaches 0, the color of the atom becomes paler.



For phenol, the greatest negative charge is on the oxygen atom. The greatest positive charge is on the adjacent carbon atom (with the adjacent hydrogen atom a close second). The rest of the molecule has relatively pale atoms; their partial charges are much closer to zero.

In addition to color, you can vary the size of atom spheres or dot surfaces by partial charge.

1. Select the Color By Element radio button in Model Display tab of the Model Settings dialog box.
2. Click the Atom Display tab.
3. Click the Show by Default checkbox in the Solid Spheres section.
4. Select the Partial Charges radio button.

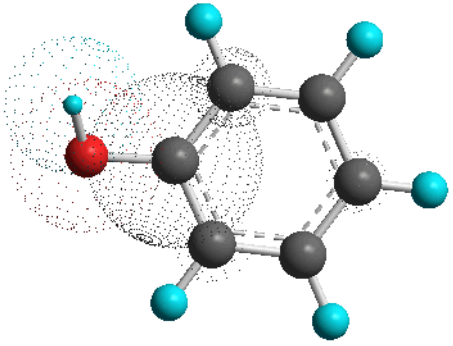


In this representation, the oxygen atom and its two adjacent atoms are large because they have relatively large partial charges of opposite signs. The rest of the atoms are relatively small.

You can display dot surfaces whose size is specified by partial charge.

1. Click the VDW Radius radio button in the Solid Spheres section.

1. Select the Show By Default check box in the Dot Surfaces section.
2. Click the Partial Charges radio button.



In this representation, the oxygen atom and its two adjacent atoms have large dot surface clouds around them because they have relatively large partial charges of opposite signs. The rest of the

atoms are relatively small. Their dot surfaces are obscured by the solid spheres. If another molecule were to react with this molecule, it would tend to react where the large clouds are, near the oxygen atom.

Chapter 3: Displaying Models

Overview

You can display molecular models in several ways, depending on what information you want to learn from them. The atoms and bonds of a model can take on different appearances. These appearances are generically termed rendering types, and the term *model display* is used in Chem3D. Depending on the type of molecule, certain model displays may offer advantages by highlighting structural features of interest. For example, the Ribbons model display might be the option of choice to show the conformational folding of a protein without the distracting structural detail of individual atoms.

Model display options are divided into two general types:

- Structure displays
- Molecular surface displays

Structure Displays

Structures are graphical representations based on the traditional physical three-dimensional molecular model types. The following structure display types are available from Model Display view of the Chem 3D Setting dialog box:

- Wire Frame
- Sticks
- Ball and Stick
- Cylindrical Bonds
- Space Filling
- Ribbons
- Cartoons

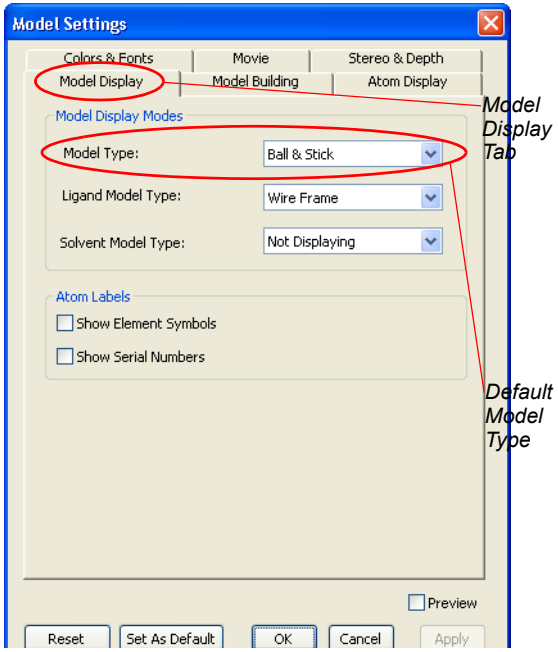
To change the default structural display type of a model:

1. From the File menu, choose Model Settings.

   The Chem 3D Setting dialog box appears.

2. Select the Model Display tab.

   The Model Display control panel of the Chem 3D Setting dialog box appears.



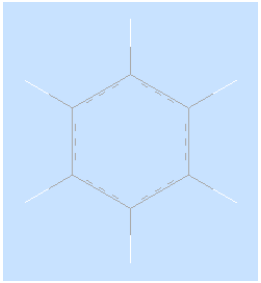
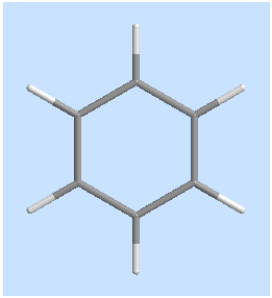
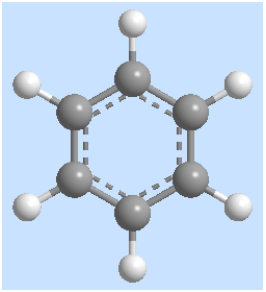
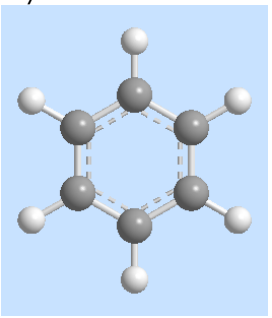
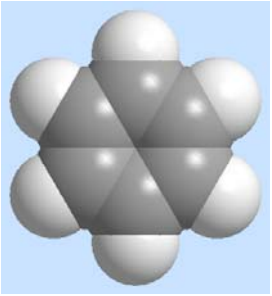
3. Set the new options.

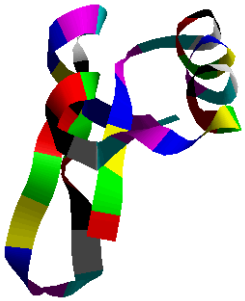
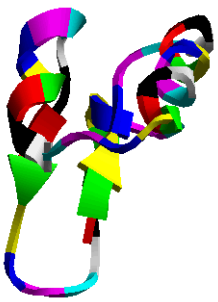
To change the structural display type of a model temporarily:

1. Click the arrow on the Model Display tool, and select the display type.

Model Types

The following table describes the Chem3D model types:

Model Type	Description
Wire Frame 	Wire Frame models are the most simple model type. Bonds are displayed as pixel-wide lines. Atoms are not displayed explicitly, but each half of a bond is colored to represent the element color for the atom at that end. Wire Frame models are well suited for extremely large models such as proteins.
Sticks 	Stick models are similar to Wire Frame, however, the bonds are slightly thicker. As this model type is also fairly fast, it is another good choice for visualizing very large models such as proteins.
Ball and Stick 	Ball and Stick models show bonds drawn as thick lines and atoms are drawn as filled spheres. The atom spheres are filled with color that corresponds to the element or position of the atom.
Cylindrical Bonds 	Cylindrical Bond models are similar to Ball and Stick models except that all bond types are drawn as cylinders.
Space Filling 	Space Filling models are more complex to draw and slowest to display. Atoms are scaled to 100% of the van der Waals (VDW) radii specified in the Atom Types table. *NOTE: The VDW radii are typically set so that overlap between non-bonded atoms in space filling models indicates a significant (approximately 0.5 kcal/mole) repulsive interaction.*

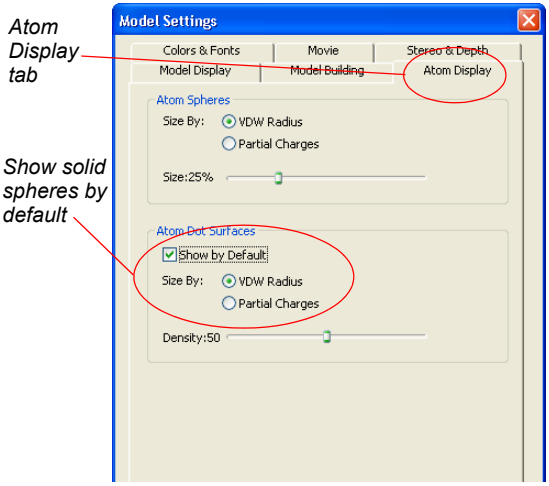
Model Type	Description
Ribbons 	Ribbons models show large protein molecules in a form that highlights secondary and tertiary structure. Ribbon models can be colored by Group to help identify the amino acid constituents. Your model must have a protein backbone in order to display ribbons.
Cartoons 	Cartoon models, like Ribbon models, show large protein molecules in a form that highlights secondary and tertiary structure. The following caveats apply to the Ribbon and Cartoon model display types: • They do not provide pop-up information. • They should be printed as bitmaps.

Displaying Solid Spheres

In Ball and Stick, Cylindrical Bond, and Space Filling models, you can display the solid spheres representing atoms and control their size.in individual atoms or all atoms.

To display solid spheres by default on all atoms:

1. From the File menu, select Model Settings.
2. Select the Atom Display tab.
3. In the Solid Spheres section, click the Show By Default checkbox.



To change the display of solid spheres in a model:

- From the Model Display submenu of the View menu, select or deselect Show Atom Dots.

Setting Solid Sphere Size

The maximum radius of the sphere that represents an atom can be based on the Van der Waals (VDW) Radius or Partial Charge. To specify which property to use, select the radio button below the slider.

The VDW Radius is specified using the atom type of the atom.

The Partial Charge is the result of a calculation: Extended Hückel, MOPAC, or Gaussian. If you have not performed a calculation, the partial charge for each atom is shown as 0, and the model will display as a Stick model. If you have performed more than one calculation, you can specify the calculation to use from the Choose Result submenu on the Calculations menu.

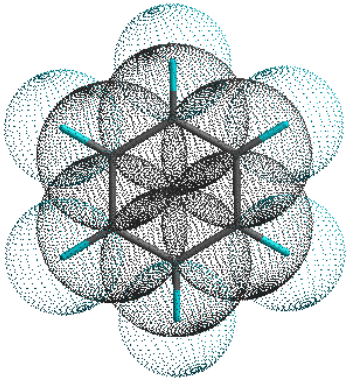
When sizing by partial charge, the absolute value of the charge is used. An atom with a partial charge of 0.500 will have the same radius as an atom with a partial charge of -0.500.

Solid Spheres Size %

The value of the Size% slider on the Atom Display tab represents a percentage of the Covalent radius specified for each atom in the Elements Table. This percentage ranges from 0 (small) to 100 (large). Thus, when the Atom Size is 100, the atoms are scaled to their maximum radii. The value of this setting affects Ball and Stick and Cylindrical Bond models.

Displaying Dot Surfaces

You can add dot surfaces to any of the model display types like the stick model shown below:



The dot surface is based on VDW radius or Partial Charges as set in the Atom Display table of the Model Settings dialog box.

To display dot surfaces by default on all atoms:

1. In the Chem 3D Model Settings dialog box, click the Atom Display tab.
2. In the Dot Surfaces area, click the Show By Default checkbox.

All atoms currently in the model window display the selected option.

You can vary the number of dots displayed in a surface by using the density slider. This is useful when dot surfaces are applied to a very small or very large models.

To change the display of dot surfaces in a model:

- From the Model Display submenu of the View menu, select or deselect Show Atom Dots.

Coloring Displays

You can change the default for the way colors are used to display your model in the Model Display tab of the Model Settings control panel. To make a temporary change, use the Color By... command on the Model Display submenu of the View menu. The choices are:

- Monochrome
- Partial Charge
- Chain
- Element
- Group
- Depth

Two of the choices, Monochrome and Chain, are only available for proteins displayed in the Ribbon or Cartoon mode.

Coloring by Element

Color by element is the usual default mode for small molecules. The default colors are stored in the Elements Table.

To change the color of elements specified in the Elements table:

1. From the View menu, point to Parameter Tables, and choose Elements.

   The Elements Table opens.
2. Double-click the Color field for an element.

   The Color dialog box appears.
3. Select the color to use and click OK.

4. Close and Save the table.

NOTE: You must save the changes before they take effect.

Coloring by Group

You may assign different colors to substructures (groups) in the model.

To change a color associated with a group in the active model:

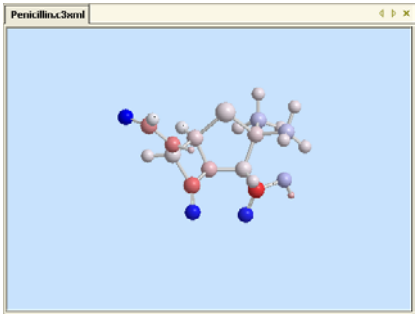
1. In the Model Explorer, Right-click on the group name and choose Select Color.

   The Color dialog box appears.
2. Select the color to use and click OK.
3. Save the changes to the Model.

Coloring by Partial Charge

When coloring by partial charge, atoms with a highly negative partial charge are deep blue. Atoms with a highly positive partial charge are deep red. As the partial charge gets closer to 0, the atom is paler. Atoms with a 0 partial charge are white.

The Partial Charge is the result of a calculation—Extended Hückel, MOPAC, or Gaussian. If you have not performed a calculation, the partial charge for each atom is 0. If you have performed more than one calculation, you can specify the calculation to use in the Choose Result submenu of the Calculations menu.



Coloring by depth for Chromatek stereo viewers

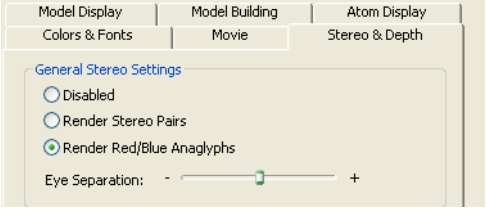
Chem3D supports color by depth for Chromadepth stereo viewers. When you select Color by Depth, the model is colored so that objects nearer the viewer are toward the red end, and objects further from the viewer toward the blue end, of the spectrum. This creates a stereo effect when viewed with a Chromadepth stereo viewer. The effect is best viewed with a dark background. If you use the Chromatek icon on the Model Display toolbar to activate this viewing option, rather than the Color By Depth menu, the background color is set automatically to black.

Red-blue Anaglyphs

Chem3D supports viewing with red-blue 3D glasses to create a stereo effect similar to that of the Chromatek viewer.

To activate red-blue viewing:

1. From the Stereo and Depth tab of the Model Settings dialog box, select Render Red/Blue Anaglyphs.
2. Move the Eye Separation slider to adjust the effect.



To toggle the effect on or off:

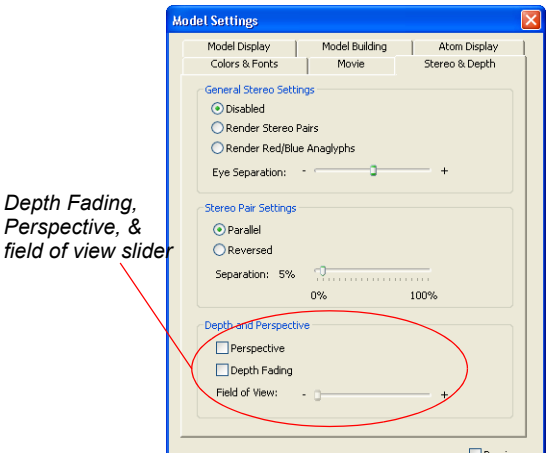
- From the Model Display submenu of the View menu, choose Red&Blue.

Depth Fading3D enhancement:

The depth fading feature in Chem3D creates a realistic depth effect, by making parts of the model further from the viewer fade into the background. Depth shading is activated by selecting the Depth Fading checkbox on the Stereo and Depth tab of the Model Settings dialog box, by selecting Depth Fading from the Model Display submenu of the View menu, or by clicking the Depth fading icon on the Toolbar.

Perspective Rendering

Chem3D supports true perspective rendering of models. This results in a more realistic depiction of the model, with bond lengths and atom sizes further from the viewer being scaled consistently. The "field of view" slider adjusts the perspective effect. Moving the slider to the right increases the effect.



CAUTION

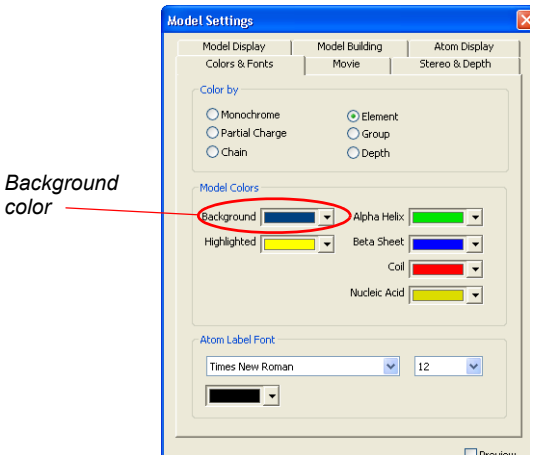
Moving the slider all the way to the left may make the model disappear completely.

Coloring the Background Window

Chem3D allows you to select a color for the background of your models. A black or dark blue background can be particularly striking for ribbon displays intended for full color viewing, whereas a light background is more suitable for print copy.

To change the default background color of the model window:

1. In the Colors and Fonts tab of the Model Settings control panel, click Background Color.



   The Color dialog box appears.

2. Select a color and click OK.

NOTE: The background colors are not saved in PostScript files or used when printing, except when you use the Ribbons display.

Coloring Individual Atoms

You can mark atoms individually using the Select Color command in the Model Explorer.

To change an atom to a new solid color:

1. In the Model Explorer, select the atom(s) to change.
2. From the Right-click menu, choose Select Color.

   The Color dialog box appears.

3. Select a color and Click OK.

   The color of the atom(s) changes to the new color.

To remove a custom atom color from the model display:

1. In the Model Explorer, select the atoms whose colors you want to change.
2. Right-click, point to Apply Atom Color and choose Inherit Atom Color.

   The custom colors are removed from the selected atoms.

Displaying Atom Labels

You can control the appearance of element symbols and serial numbers using the Atom Labels tab in the Model Settings control panel, and the corresponding commands in the Model Display submenu of the View menu.

Setting Default Atom Label Display Options

To set the Element Symbols and Serial Numbers defaults:

1. On the Colors and Fonts tab of the Model Settings dialog box, select the font, point size and color.
2. Click the Set as Default button.

   All atoms currently in the model window display the selected options.

To toggle the Atom Labels or Serial Numbers at any time, do one of the following:

- From the Model Display submenu of the View menu, choose Show Atom Labels or Show Serial Numbers.
- Click the Atom Label or Serial Numbers icon on the Model Display Toolbar.

Displaying Labels Atom by Atom

To display element symbols or serial numbers in individual atoms:

1. In the Model Explorer, select the atom to change.
2. On the Right-click menu, point to Atom Serial Number or Atom Symbol and choose Show...

Using Stereo Pairs

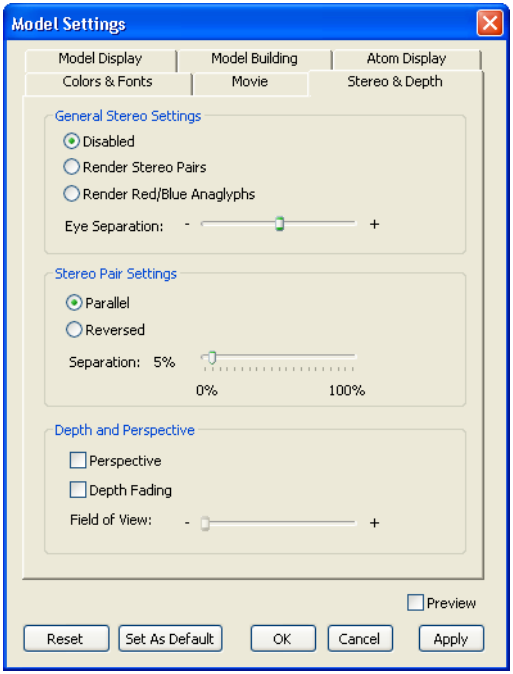
Stereo Pairs is a display enhancement technique based on the optical principles of the Stereoscope, the late-Nineteenth century device for 3D viewing of photographs. By displaying two images with a slight displacement, a 3D effect is created.

Stereo views can be either Parallel or Reverse (direct or cross-eyed). Some people find it easier to look directly, others can cross their eyes and focus on two images, creating an enhanced three dimensional effect. In either case, the effect may be easier to achieve on a printed stereo view of your model than on the screen. Keep the images relatively small, and adjust the distance from your eyes.

To set the Stereo Pairs parameters:

1. Open the Model Setting dialog box, and click the Stereo and Depth tab.

   The stereo views control panel appears.



2. Select Render Stereo Pairs to display two views of the model next to each other.

   The right view is the same as the left view, rotated about the Y-axis.

3. Specify the Eye Separation (Stereo Offset) with the slider. This controls the amount of Y-axis rotation.

4. Specify the degree of separation by clicking the Separation arrows.

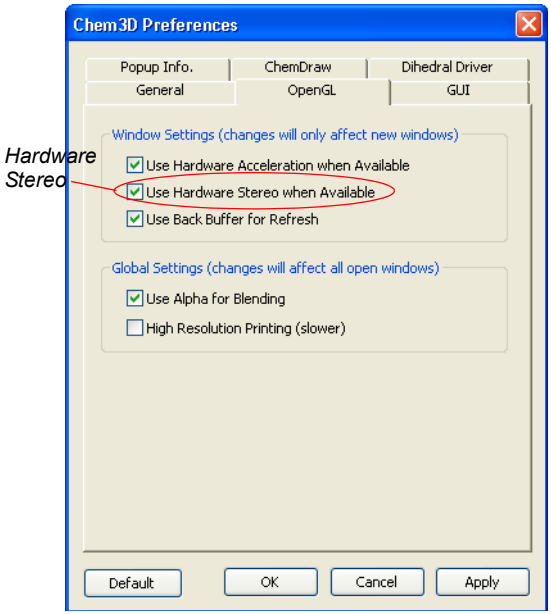
   About 5% of the width is a typical separation for stereo viewing.

To select whether the views are cross-eyed or direct, do one of the following:

- Select Reverse to rotate the right frame to the left. If your left eye focuses on the right-hand model and your right eye focuses on the left-hand model, the two stereo views can overlap.
- Select Parallel to rotate the right view further to the right.

Using Hardware Stereo Graphic Enhancement

Chem3D 9.0 provides stereo graphics rendering for hardware that has stereo OpenGL capabilities. There are now a variety of stereo graphics cards, stereo glasses, and 3D monitors that can be driven by Chem3D. Hardware enhancement is enabled from the OpenGL tab in the Chem3D Preferences dialog, which you can access from the File menu.

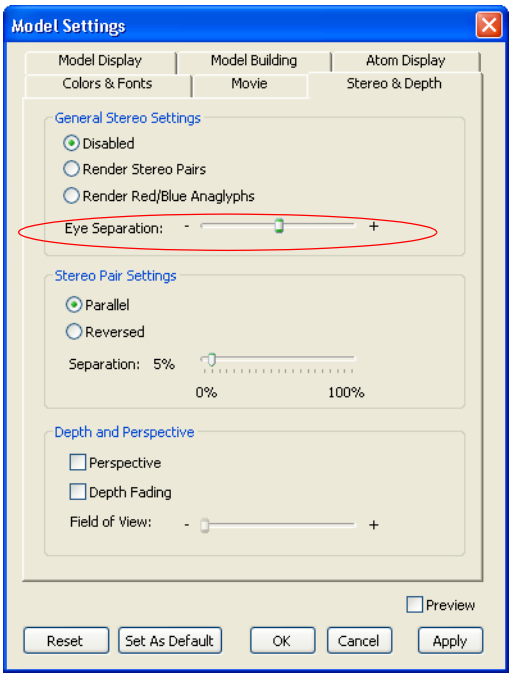


Any 3D window opened after this mode is enabled will utilize hardware graphics capabilities if they are available and enabled.

NOTE: You must enable "stereo in OpenGL" in the display adapter properties control, as well as in Chem3D preferences, and select the correct mode for the glasses/ monitor you are using.

You can use depth fading and perspective with hardware enhancement, but should not activate other stereo modes.

TIP: The Eye Separation *slider on the* Stereo and Depth *tab of the Model Settings dialog box can be used to control separation. You should select the* Disabled *radio button when using hardware stereo.*



Molecular Surface Displays

Molecular Surface displays provide information about entire molecules, as opposed to the atom and bond information provided by Structure displays. Surfaces show information about a molecule's physical and chemical properties. They display aspects of the external surface interface or electron distribution of a molecule.

Unlike atom and bond data, Molecular Surface information applies to the entire molecule. Before any molecular surface can be displayed, the data necessary to describe the surface must be calculated using Extended Hückel or one of the methods available in CS MOPAC or Gaussian. Under MOPAC you must choose Molecular Surfaces as one of the properties to be calculated.

There is one exception to the requirement that you must perform a calculation before a molecular surface can be displayed. Solvent Accessible surfaces are automatically calculated from parameters stored in the Chem3D parameters tables. Therefore, no additional calculations are needed, and the Solvent Accessible command on the Choose Surface submenu is always active.

Extended Hückel

Extended Hückel is a semi-empirical method that can be used to generate molecular surfaces rapidly for most molecular models. For this reason, a brief discussion of how to perform an Extended Hückel calculation is given here. For more information, see Appendix 8: "Computation Concepts".

To compute molecular surfaces using the Extended Hückel method:

- From the Computations menu, point to Extended Hückel, and choose Calculate Surfaces.

NOTE: Before doing an Extended Hückel calculation, Chem3D will delete all lone pairs and dummy atoms. You will see a message to this effect in the Output window.

At this point, a calculation has been performed and the results of the calculation are stored with the model.

To compute partial charges using the Extended Hückel method:

- From the Computations menu, point to Extended Hückel, and choose Calculate Charges.

For each atom in the model, a message is created listing the atom and its partial charge. If you have selected Partial Charge in the Pop-up Information tab of the Model Settings dialog box, then the partial charges will appear as part of the pop-up information when you point to an atom.

Displaying Molecular Surfaces

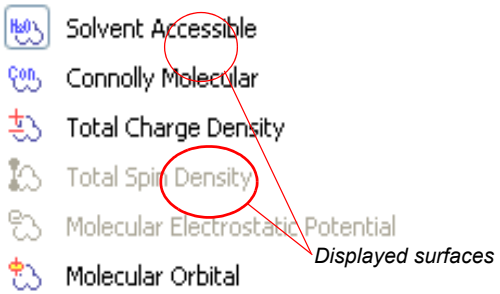
To display a surface:

1. Decide what surface type to display.
2. Perform a suitable calculation using Extended Hückel, CS MOPAC, or Gaussian 03. Include the Molecular Surfaces property calculation whenever it is available.

   NOTE: **Ultra** *CS MOPAC and Gaussian 03 surfaces calculations are only available in Chem3D Ultra.*

   Different calculation types can provide different results. If you have performed more than one calculation on a model, for example, both an Extended Hückel and an AM1 calculation, you must choose which calculation to use when generating the surface.
3. From the Calculations menu, point to Choose Result and select one of your calculations.
4. From the Surfaces menu point to Choose Surface, and select one of the surface types.

   NOTE: The Choose Surface commands are toggle switches–click once to display, click again to turn off the display. You can display more than one surface at a time. When a surface is displayed, its icon is highlighted with a light blue background.



5. Adjust the display using the surface display tools.

   TIP: If you are making a lot of adjustments to the display, activate the Surfaces toolbar and tear off the specific tools you will be using often.

For a review of the surface display tools, see "The Surfaces Toolbar" on page 21.

Not all surfaces can be displayed from all calculations. For example, a Molecular Electrostatic Potential surface may be displayed only following a Gaussian or MOPAC calculation. If a surface is unavailable, the command is grayed out in the submenu.

To generate surfaces from MOPAC or Gaussian, you must choose Molecular Surfaces as one of the properties calculated by these programs. The surface types and the calculations necessary to display them are summarized in the following table.

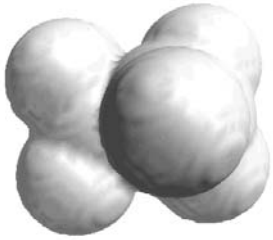
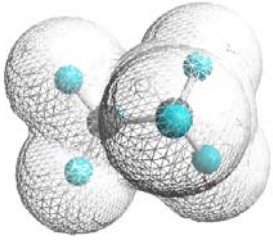
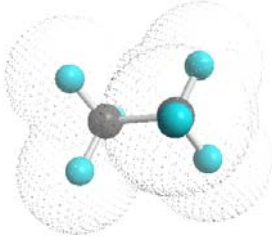
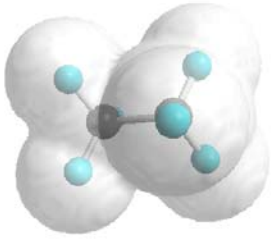
NOTE: Spin Density map requires that MOPAC or Gaussian computations be performed with an open shell wavefunction.

Surface Type	**Extended Hückel**	**MOPAC**	**Gaussian**
Solvent Accessible[a]	NA	NA	NA
Connolly Molecular	Yes	Yes	Yes
Total Charge Density	Yes	Yes	Yes
with Molecular Orbital map	Yes	Yes	Yes
with Spin Density map	No	Yes	Yes
with Partial Charges	Yes	Yes	Yes
with Molecular Electrostatic Potential map	No	Yes	Yes
Total Spin Density	No	Yes	Yes
Molecular Electro-static Potential	No	Yes	Yes
Molecular Orbitals	Yes	Yes	Yes

a. Calculated automatically from parameters stored in the Chem3D parameters tables. This surface is always available with no further calculation.

Setting Molecular Surface Types

Chem3D offers four different types of surface displays, each with its own properties. These types are shown in the following table:

Surface Type	Description
Solid 	The surface is displayed as an opaque form. Solid is a good choice when you are interested in the details of the surface itself, and not particularly interested in the underlying atoms and bonds.
Wire Mesh 	The surface is displayed as a connected net of lines. Wire Mesh is a good choice when you want to focus on surface features, but still have some idea of the atoms and bonds in the structure.
Dots 	The surface is displayed as a series of unconnected dots. Dots are a good choice if you are primarily interested in the underlying structure and just want to get an idea of the surface shape.
Translucent 	The surface is displayed in solid form, but is partially transparent so you can also see the atoms and bonds within it. Translucent is a good compromise between surface display styles.

Setting Molecular Surface Isovalues

Isovalues are, by definition, constant values used to generate a surface. For each surface property, values can be calculated throughout space. For example, the electrostatic potential is very high near each atom of a molecule, and vanishingly small far away from it. Chem3D generates a surface by connecting all the points in space that have the same value, the ***isovalue***. Weather maps are a common example of the same procedure in two dimensions, connecting locations of equal temperature (isotherms) or equal pressure (isobars).

To set the isovalue:

1. From the Surfaces menu, choose Isocontour.

   NOTE: The exact name of this command reflects the type of isovalue in each window. For example, for Total Charge Density Surfaces, it is "Isocharge".

   The Isocontour slider appears.

2. Adjust the slider to the new isovalue.

   The new isovalue is the middle value listed at the bottom of the Isocontour tool.

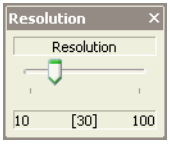
Setting the Surface Resolution

The Surface Resolution is a measure of how smooth the surface appears. The higher the resolution, the more points are used to calculate the surface, and the smoother the surface appears. However, high resolution values can also take a long time to calculate. The default setting of 30 is a good compromise between speed and smoothness.

To set the resolution:

1. From the Surfaces menu, choose Resolution.

   The Resolution slider appears.



2. Adjust the slider to the desired resolution.

   The new resolution is the middle value listed at the bottom of the Resolution tool.

Setting Molecular Surface Colors

How you set the color depends on what type of surface you are working with.

For Solvent Accessible, Connolly Molecular, or Total Charge Density surfaces, do the following:

1. On the Surfaces menu, choose Surface Color.

   The Surface Color dialog box appears.
2. Select the new color.
3. Click OK.

For the other surface types, where you must specify two colors, do the following.

1. On the Surfaces menu, choose Alpha Color or Beta Color.

   The Alpha or Beta Color dialog box appears.
2. Select the new color.
3. Click OK.

Setting Solvent Radius

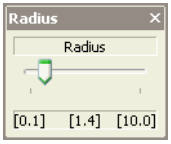
The Solvent Radius can be set from 0.1 to 10 Å using the slider. The default solvent radius is 1.4 Å, which is the value for water. Radii for some common solvents are shown in the following table:

Solvent	Radius (Å)
Water	1.4
Methanol	1.9
Ethanol	2.2
Acetonitrile	2.3
Acetone	2.4
Ether	2.4
Pyridine	2.4
DMSO	2.5
Benzene	2.6
Chloroform	2.7

To set the solvent radius:

1. From the Surfaces menu, choose Solvent Radius.

   The Radius slider appears.



2. Adjust the slider to the desired resolution.

   The new radius is the middle value listed at the bottom of the Radius tool.

Setting Surface Mapping

The Mapping Property provides color-coded visualization of Atom Colors, Group Colors, Hydrophobicity, Partial Charges, or Electrostatic Potential (derived from partial charges) superimposed upon the solvent-accessible surface.

Surface Color is color you have chosen with the Surface Color tool. **Atom Color** is based on the displayed atom colors, which may or may not be the default element colors. **Element Color** is based on the default colors in the Elements Table. **Group Color** is based on the colors (if any) you specified in the Model Explorer when creating groups.

Hydrophobicity is displayed according to a widely-used color convention derived from amino acid hydrophobicities[1], where the most hydrophobic (lipophilic) is red and the least hydrophobic (lipophobic) is blue. The following table shows molecule hydrophobicity.

Amino Acid	Hydrophobicity	
Phe	3.7	Most hydrophobic (Red)
Met	3.4	
Ile	3.1	
Leu	2.8	
Val	2.6	
Cys	2.0	
Trp	1.9	
Ala	1.6	
Thr	1.2	
Gly	1.0	
Ser	0.6	Middle (White)
Pro	–0.2	
Tyr	–0.7	
His	–3.0	
Gln	–4.1	
Asn	–4.8	
Glu	–8.2	
Lys	–8.8	
Asp	–9.2	
Arg	–12.3	Least hydrophobic (Blue)

1. Engelman, D.M.; Steitz, T.A.; Goldman, A., "Identifying nonpolar transbilayer helices in amino acid sequences of membrane proteins", *Annu. Rev. Biophys. Biophys. Chem.* **15**, 321-353, 1986.

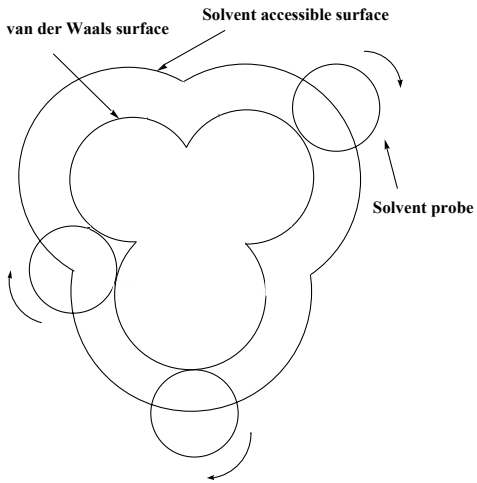
The **Partial Charges** and **Electrostatic Potential** (derived from the partial charges) properties are taken from the currently selected calculation. If you have performed more than one calculation on the model, you can specify which calculation to use from the Choose Result submenu of the Calculations menu.

Solvent Accessible Surface

The solvent accessible surface represents the portion of the molecule that solvent molecules can access. When viewed in the ball and stick representation, a molecule may appear to have many nooks and crannies, but often these features

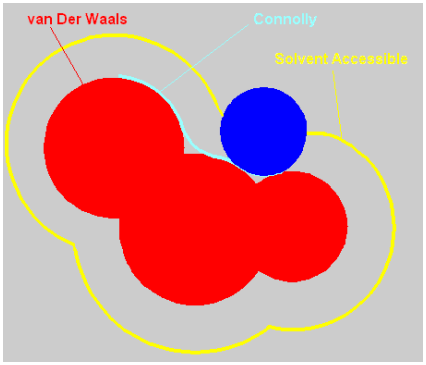
are too small to affect the overall behavior of the molecule. For example, in a ball-and-stick representation, it might appear that a water molecule could fit through the big space in the center of a benzene molecule. The solvent accessible surface (which has no central hole) shows that it cannot. The size and shape of the solvent accessible surface depends on the particular solvent, since a larger solvent molecule will predictably enjoy less access to the crevices and interstices of a solute molecule than a smaller one.

To determine the solvent-accessible surface, a small probe sphere simulating the solvent molecule is rolled over the surface of the molecule (van der Waals surface). The solvent-accessible surface is defined as the locus described by the center of the probe sphere, as shown in the diagram below.

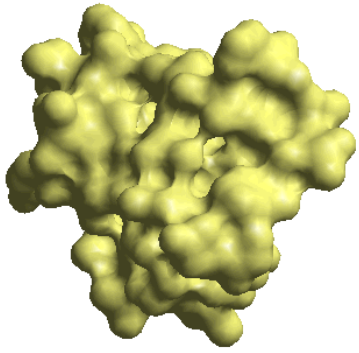


Connolly Molecular Surface

The Connolly surface, also called the molecular surface, is similar to the solvent-accessible surface. Using a small spherical probe to simulate a solvent, it is defined as the surface made by the center of the solvent sphere as it contacts the van der Waals surface. The volume enclosed by the Connolly surface is called the solvent-excluded volume. These surfaces are shown in the following illustration.



The Connolly Surface of icrn is shown below:



ULTRA Total Charge Density

The Total Charge Density is the electron density in the space surrounding the nuclei of a molecule, or the probability of finding electrons in the space around a molecule. The default isocharge value of 0.002 atomic units (a.u.) approximates the molecule's van der Waals radius and represents about 95% of the entire three-dimensional space occupied by the molecule.

The Total Charge Density surface is the best visible representation of a molecule's shape, as determined by its electronic distribution. The Total Charge

Density surface is calculated from scratch for each molecule. The Total Charge Density is generally more accurate than the Space Filling display.

For Total Charge Density surfaces, the properties available for mapping are Molecular Orbital, Spin Density, Electrostatic Potential, and Partial Charges. The color scale uses red for the highest magnitude and blue for the lowest magnitude of the property. Neutral is white.

You can choose the orbital to map onto the surface with the Molecular Orbital tool on the Surfaces menu. The orbital number appears in parentheses in the HOMO/LUMO submenu.

[ULTRA] Total Spin Density

The total spin density surface describes the difference in densities between spin-up and spin-down electrons in any given region of a molecule's space. The larger the difference in a given region, the more that region approximates an unpaired electron. The relative predominance of spin-up or spin-down electrons in regions of the total spin density surface can be visualized by color when total spin density is mapped onto another surface (total charge density). Entirely spin-up (positive value) electrons are red, entirely spin-down (negative) blue, and paired electrons (neutral) are white.

The total spin density surface is used to examine the unpaired electrons of a molecule. The surface exists only where unpaired electrons are present. Viewing the total spin density surface requires that both Spin Density and Molecular Surfaces are calculated by MOPAC or Gaussian using an Open Shell Wavefunction.

[ULTRA] Molecular Electrostatic Potential

The molecular electrostatic potential (MEP) represents the attraction or repulsion between a molecule and a proton. Attraction is represented by negative values and repulsion is indicated by positive values. Experimental MEP values can be obtained by X-ray diffraction or electron diffraction techniques, and provide insight into which regions of a molecule are more susceptible to electrophilic or nucleophilic attack. You can visualize the relative MEP values by color when MEP is mapped onto another surface (total charge density). The most positive MEP value is red, the most negative blue, and neutral is white.

Molecular Orbitals

Molecular orbital (MO) surfaces visually represent the various stable electron distributions of a molecule. According to frontier orbital theory, the shapes and symmetries of the highest-occupied and lowest-unoccupied molecular orbitals (HOMO and LUMO) are crucial in predicting the reactivity of a species and the stereochemical and regiochemical outcome of a chemical reaction.

To set the molecular orbital being displayed:

- From the Surfaces menu, point to Molecular Orbital to see the HOMO/LUMO options. Select the orbital.

You can specify the isocontour value for any computed MO surface using the Isocontour tool on the Surfaces menu. The default isocontour value for a newly computed surface is the value you last specified for a previously computed surface. If you have not specified an isocontour value, the default value is 0.01.

NOTE: The default isocontour value for an MO surface imported from a cube file is 0.01 regardless of any previously set isocontour value.

Visualizing Surfaces from Other Sources

You can use files from sources other than Chem3D to visualize surfaces. From Windows sources, you can open a Gaussian Formatted Checkpoint (.fchk) or Cube (.cub) file.

From sources other than Windows, create a Gaussian Cube file, which you can open in Chem3D.

Chapter 4: Building and Editing Models

Overview

Chem3D enables you to build or change a model by three principal methods:

- Using the ChemDraw panel, which utilizes ChemDraw to build and insert or copy and edit models.
- Using Bond tools, which build using carbon exclusively.
- Using the Build from Text tool (hereafter referred to as the Text tool), which allows you to build or edit models using atom labels and substructures.

Usually, a combination of methods yields the best results. For example, you might build a carbon skeleton of a model with ChemDraw or the bond tools, and then change some of the carbons into other elements with the Text tool. Or you can build a model exclusively using the Text tool.

In addition, you can use Structure tools to change bond lengths and angles, or to change stereochemistry.

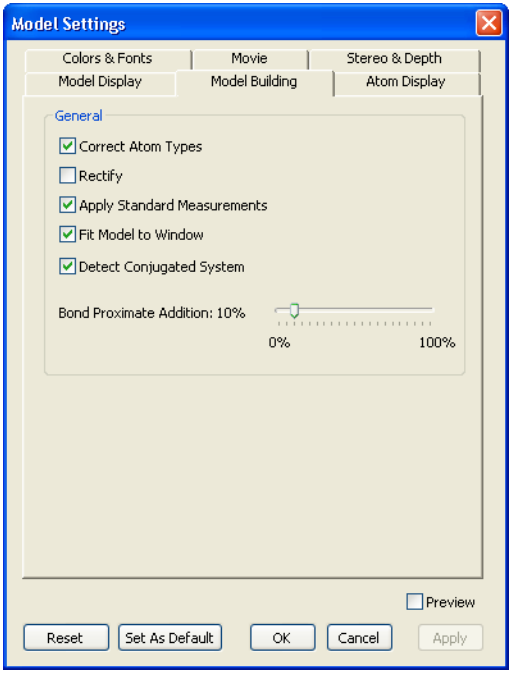
Setting the Model Building Controls

You control how you build by changing options in the Building control panel in the Model Settings dialog box. The default mode is all options selected. You can choose to build in a faster mode, with less built-in "chemical intelligence", by turning off one or more of the options.

Intelligent mode yields a chemically reasonable 3D model as you build. Fast mode provides a quick way to generate a backbone structure. You can then turn it into a chemically reasonable 3D model by using the Structure menu Rectify and Clean Up tools.

To change the Building mode:

1. From the File menu, choose Model Settings.
   The Model Settings dialog box appears.
2. Select the Model Building tab.



3. Select or deselect the appropriate radio buttons.

The following table describes the Model Build controls

Control	Description
Correct Atom Types	Determines whether atom types are assigned to each atom as you build. Atom types, such as "C Alkane" specify the valence, bond lengths, bond angles, and geometry for the atom.
Rectify	Determines whether the open valences for an atom are filled, usually with hydrogen atoms.
Apply Standard Measurements	Determines whether the standard measurements associated with an atom type are applied as you build.
Fit Model to Window	Determines whether the entire model is resized and centered in the model window after a change to the model is made.
Detect Conjugated System	When selected, all bonds in a conjugated system are set at a bond order of 1.5. When unselected, bonds are displayed as drawn. Does not affect previously drawn structures.
Bond Proximate Addition (%)	Determines whether a bond is created between a selection of atoms. For more information see "Creating Bonds by Bond Proximate Addition" on page 84.

NOTE: *For more information about atom types, standard measurements, and rectification, see "Model Building Basics" on page 24.*

Building with the ChemDraw Panel

Chem3D 9 makes it easier than ever to create or edit models in ChemDraw. The ChemDraw panel is activated from the View menu. Using ActiveX technology, it puts the functionality of ChemDraw Pro at your fingertips.

To add a new structure to Chem3D:

1. Open the ChemDraw Panel by selecting it from the View menu.

   The ChemDraw panel appears on the right of the model window.
2. Click in the panel to activate it.

   The Tools palette appears.

   TIP: *If you don't see the Tools palette, right-click in the ChemDraw panel, and check the View menu to see that it has been activated. There should be a check mark next to* Show Main Tools. *While you are at it, you might want to activate other toolbars. Activating the General tools toolbar, for example, will give you access to undo/redo commands.*
3. Build the structure.

   The model appears simultaneously in both the ChemDraw and Chem3D model windows.

Unsynchronized Mode

By default, the ChemDraw panel works in synchronized mode. In this mode, your model appears simultaneously in the ChemDraw panel

and in Chem3D. Editing either model changes the other automatically. This affords maximum editing flexibility.

To turn off synchronized mode:

- Click the Synch button at the top left of the ChemDraw panel. The button toggles synchronization on and off.

  To copy a model to Chem3D, click either the Add or Replace icon.

Name=Struct

The ChemDraw panel has a Name=Struct window that allows you to build models by entering a chemical name or SMILES string. You can also copy names or SMILES strings from other documents and paste them, either into the Name=Struct window, or directly into the Chem3D model window.

TIP: *You can also paste chemical formulas into the Chem3D model window. Be aware, however, that a formula may not represent a unique structure, and the results may not be correct.*

Building with Other 2D Programs

You can use other 2D drawing packages, such as ISIS/Draw to create chemical structures and then copy them into Chem3D for automatic conversion to a 3D model.

To build a model with 2D drawings:

1. In the source program, copy the structure to the clipboard.
2. In Chem3D, from the Edit menu, choose Paste.

   The 2D structure is converted to a 3D model. The standard measurements are applied to the structure. For more information see "Appendix D: 2D to 3D Conversion."

NOTE: *You cannot paste from ISIS/Draw into the ChemDraw panel, only into the Chem3D model window. You can, however use the synchronize control to add the model to the ChemDraw panel.*

You can also cut-and-paste, or drag-and-drop, models to and from ChemDraw to Chem3D or the ChemDraw panel. See "Transferring to Other Applications" on page 127 for more information on pasting into other applications.

Non-bond or atom objects copied to the clipboard (arrows, orbitals, curves) are ignored by Chem3D. Superatoms in ISIS/Draw are expanded if Chem3D finds a corresponding substructure. If a corresponding structure is not found, you must define a substructure. For more information see "Defining Substructures" on page 232.

Building With the Bond Tools

Use the bond tools to create the backbone structure of simple models. Bond tools always create bonds that terminate with carbon atoms. Hydrogens display automatically by default. You can hide them to reduce clutter. You can change the carbons or hydrogens to other elements after you create the generic model.

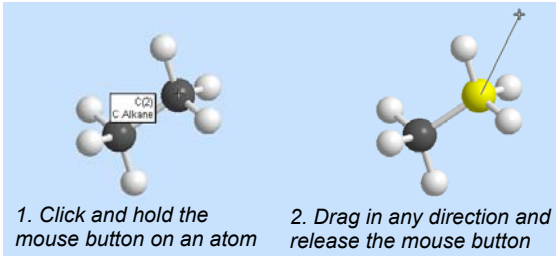
To create a model using a Bond tool:

1. Choose a bond tool. The Single Bond tool is used in this example.
2. Point in the model window, and drag in the direction you want the bond to be oriented.
3. Release the mouse button to complete the bond.

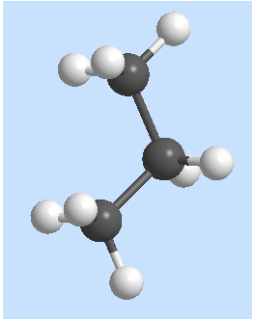
When Correct Atom Types and Rectify settings are selected in the Building control panel, the atom type is set according to the bond tool used (C Alkane in this example) and the appropriate number of hydrogens are added.

To add bonds to the model:

4. Point to an atom and drag in the direction you want to create another atom.



When the Rectify option is set in the Building control panel, the hydrogen is replaced by a carbon.



5. Repeat adding bonds until you have the model you want.

   After you have the backbone, you can change the carbons to different heteroatoms.

Creating Uncoordinated Bonds

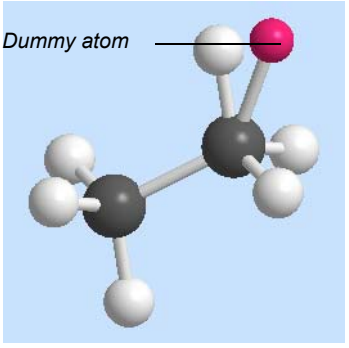
Use the Uncoordinated Bond tool to create an uncoordinated bond with a dummy atom (labeled Du). Uncoordinated Bonds and dummy atoms are ignored in all computations. An uncoordinated bond allows you to specify a connection between two atoms without a strict definition of the type of bond. This bond is often used in coordination complexes for inorganic compounds, where another element might be substituted.

Dummy atoms are also useful for positioning atoms in a Z-matrix, perhaps for export to another application for further analysis. This is a common use when models become large and connectivities are difficult to specify.

To add an uncoordinated bond and dummy atom:

1. Select the Uncoordinated Bond tool .
2. Point to an atom and drag from the atom.

   An uncoordinated bond and a dummy atom are added to the model. The atom created is labeled "Du", the Chem3D element symbol for Dummy atoms.



Removing Bonds and Atoms

When you remove bonds and atoms:

- Click a bond to remove only that bond.
- Click an atom to remove the atom and all attached bonds.

To remove an atom or bond, do one of the following:

- Click the Eraser tool and click the atom or bond.

- Select the atom or bond, and from the Edit menu, choose Clear.
- Select the atom or bond and press Delete.

NOTE: *If automatic rectification is on, you will not be able to delete hydrogen atoms. Turn rectification off when editing a model.*

Building With The Text Tool

The Text tool allows you to enter text that represents elements, atom types (elements with specific hybridization), substructures, formal charges, and serial numbers. The text you enter must be found in either the Elements, Atom Types, or Substructures tables. The match must be exact, including correct capitalization. These tables can be found in the Parameter Tables list on the View menu.

NOTE: *For all discussions below,* ***all*** *the Building control panel options in the Chem 3D Setting dialog box are assumed to be turned on.*

Some general rules about using the Text Tool are as follows:

- Text is case sensitive. For example, the correct way to specify a chlorine atom is Cl. The correct way to specify the phenyl group substructure is to type Ph. PH or ph will not be recognized.
- Pressing the Enter key applies the text to the model.
- Typing a formal charge directly after an element symbol will set the formal charge for that atom. For example PhO- will create a model of a phenoxide ion instead of phenol.
- If you double click an atom, the contents of the previous text box are applied to that atom. If the atom is one of several selected atoms, then the contents of the previous text box are applied to all of the selected atoms.
- If a tool other than the Text tool is selected, double-clicking in the model window is equivalent to clicking with the Text tool selected. Triple-clicking in the model window is equivalent to double-clicking with the Text tool selected.

The interpretation of the text in a text box depends on whether atoms are selected as follows:

- If the model window is empty, a model is built using the text.
- If you have one or more atoms selected, the text is added to the model at that selection if possible. If the specifications for a selected atom are violated, the connection cannot be made.
- If you have a model in the window, but do not have anything selected, a second fragment is added, but is not connected to the model.
- When a text box is visible, you can modify the selection by Shift+clicking or Shift-dragging across atoms.

Using Labels

To use an element symbol in a text box:

1. Select the Text tool.
2. Click in the model window.

   A text box appears.
3. Type C.
4. Press the Enter key.

   A model of methane appears.

   The atom type is automatically assigned as a C Alkane, and the appropriate number of hydrogens are automatically added.

To use the same text to add another methyl group:

1. Point to the atom you want to replace, in this example a hydrogen, and click.

   The text box appears with the previous label.
2. Press the Enter key.

To add a different element:

1. Click a hydrogen atom.

   A text box appears over the atom.
2. Type N.
3. Press the Enter key.

   A nitrogen is added to form ethylamine.

To build ethylamine in one step:

1. Click in the model window.

   A text box appears.
2. Type CH3CH2NH.
3. Press the **Enter** key.

   A model of ethylamine appears.

Changing atom types

You can use a text box to change the atom type and bonding characteristics.

To change the atom type of some atoms:

1. Click a carbon atom.

   A text box appears.
2. Shift+click the other carbon atom.

   Both atoms are selected.
3. Type C Alkene.
4. Press the Enter key.

   The atom type and the bond order are changed to reflect the new model of ethyleneamine. You can point at the atoms and bonds to display this new information.

The Table Editor

To use the Table Editor to enter text in a text box:

1. From the View menu, point to Parameter Tables, and choose Atom Types.
2. Select the element or atom type in the table.
3. From the Edit menu, choose Copy.
4. Double-click in the Chem3D Model Window.
5. In Chem3D, from the Edit menu, choose Paste.

   The copied text appears in the text box.

Specifying Order of Attachment

In both the simple and complex forms for using the Text tool, you can specify the order of attachment and repeating units by numbers and parentheses.

For example:

- Type (CH3)3CNH2 into a text box with no atoms selected and press the Enter key.

  A model of tert-butylamine appears.

Using Substructures

You can use pre-defined functional groups called substructures to build models. Some advantages for using substructures in your model building process are as follows:

- Substructures are energy minimized.
- Substructures have more than one attachment atom (bonding atom) pre-configured.

  For example, the substructure Ph for the phenyl group has a single attachment point. The substructure COO for the carboxyl group has attachment points at both the Carboxyl carbon and the Alcohol Oxygen. These provide for insertion of this group within a model. Similar multi-bonding sites are defined for all amino acid and other polymer units.

- Amino Acid substructures come in both alpha (indicated by the amino acid name alone) and beta (indicated by a ß- preceding the name of the amino acid) forms. The dihedral angles have been preset for building alpha helix and beta sheet forms.
- You can use substructures alone or in combination with single elements or atom types.
- Using a substructure automatically creates a record in the Groups table that you can use for easy selection of groups, or coloring by group.
- Substructures are particularly useful for building polymers.
- You can define your own substructures and add them to the substructures table, or create additional tables. For more information, see "Defining Substructures" on page 232.

To view the available substructures:

- From the View menu, point to Parameter Tables, and choose Substructures.

Building with Substructures

You must know where the attachment points are for each substructure to get meaningful structures using this method. Pre-defined substructures have attachment points as defined by standard chemistry conventions. For more information see "Attachment point rules" on page 231.

To use a substructure as an independent fragment, make sure there are no atoms selected.

To insert a substructure into a model, select the atoms which are bonded to the attachment points of the substructure.

To build a model using a substructure:

1. Type the name of the substructure into a text box (or copy and paste it from the Substructures table).
2. Press the **Enter** key.

   The substructure appears in the model window.

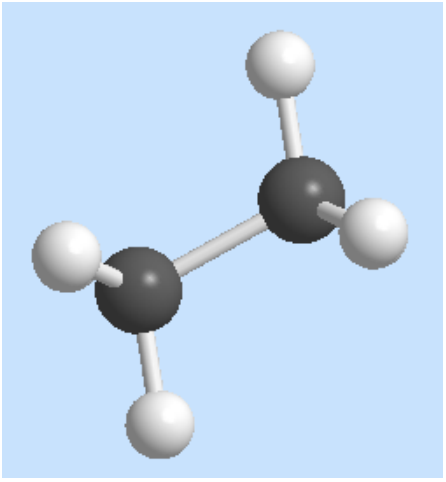
When you replace an atom or atoms with a substructure, the atoms which were bonded to the replaced atoms are bonded to the attachment points of the substructure. The attachment points left by the replaced atoms are also ordered by serial number.

Example 1. Building Ethane with Substructures

To build a model of ethane using a substructure:

1. Type Et or EtH into a text box with no atoms selected.
2. Press the Enter key.

   A model of ethane appears.



NOTE: *When automatic rectification is on, the free valence in the ethyl group is filled with a hydrogen. If automatic rectification is off, you need to type* EtH *to get the same result. For substructures with more than one atom with an open valence, explicitly specify terminal atoms for each open valence.*

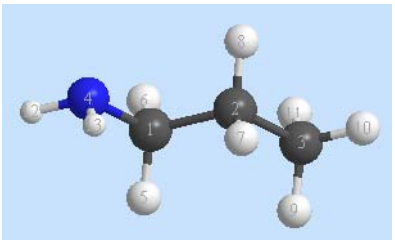
Example 2. Building a Model with a Substructure and Several Other Elements

To build a model with substructures and other elements:

1. Type PrNH2 into a text box with no atoms selected.
2. Press the Enter key.

   A model of propylamine appears.

   The appropriate bonding site for the Pr substructure is used for bonding to the additional elements NH2.



Example 3. Polypeptides

Use substructures for building polymers, such as proteins:

1. Type HAlaGlyPheOH into a text box with no atoms selected.

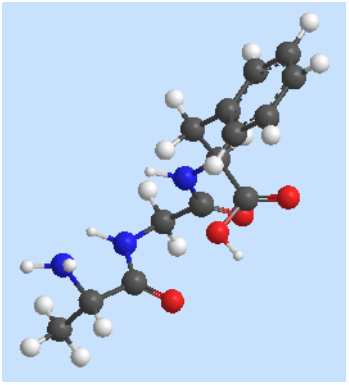
   The additional H and OH cap the ends of the polypeptide. If you don't cap the ends and automatic rectification is on, Chem3D tries to fill the open valences, possibly by closing a ring.
2. Press the Enter key.

   Ring closing bonds appear whenever the text in a text box contains two or more open valences.

The alpha form of the neutral polypeptide chain composed of Alanine, Glycine, and Phenylalanine appears.

NOTE: *You can use the amino acid names preceded with a* ß– *to obtain the beta conformation, for example* Hß–Alaß–Glyß–PheOH. *To generate the* ß *character, type Alt+0223 using the number pad.*

The appropriate bonding and dihedral angles for each amino acid are pre-configured in the substructure.



TIP: *To better view the alpha helix formation, use the Trackball Tool to reorient the model to an end-on view. For more information see "Trackball Tool" on page 97.*

To change the polypeptide to a zwitterion:

1. Select the Text tool.
2. Click the terminal nitrogen.

   A text box appears over the nitrogen atom.
3. Type + and press the Enter key.

   The charge is applied to the nitrogen atom. Its atom type changes and a hydrogen atom is added.
4. Click the terminal oxygen.

   A text box appears over the oxygen atom.
5. Type - in the text box and press the **Enter** key.

The charge is applied to the oxygen atom. Its atom type changes and a hydrogen atom is removed.

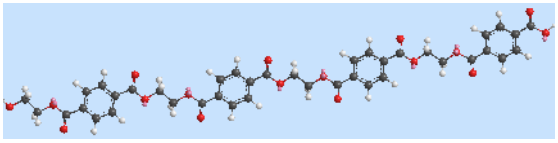
For amino acids that repeat, put parentheses around the repeating unit plus a number rather than type the amino acid repeatedly. For example, type HAla(Pro)10GlyOH.

Example 4. Other Polymers

The formation of a PET (polyethylene terephthalate) polymer with 4 units (a.k.a.: Dacron, Terylene, Mylar) ia shown below:

- Type OH(PET)4H into a text box with no atoms selected and press the Enter key.

  The H and OH are added to cap the ends of the polymer.



Replacing an Atom with a Substructure

The substructure you use must have the same number of attachment points as the atom you are replacing. For example, if you try to replace a carbon in the middle of a chain with an Ethyl substructure, an error occurs because the ethyl group has only one open valence and the selected carbon has two.

To replace an individual atom with a substructure:

1. Click the Text tool.
2. Click the atom to replace.

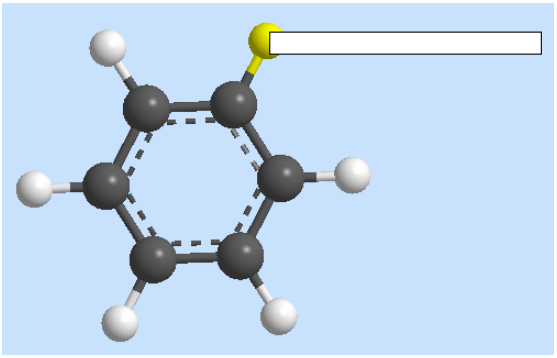
   A text box appears.
3. Type the name of the substructure to add (case-sensitive).
4. Press the Enter key.

   The substructure replaces the selected atom.

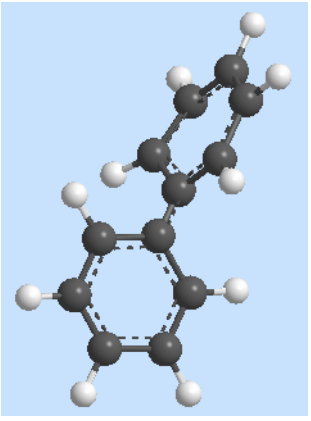
For example, to change benzene to biphenyl:

1. Click the atom to replace.

   A text box appears.



2. Type Ph.
3. Press the Enter key.



Building From Tables

Cartesian Coordinate tables and Z-Matrix tables can be saved as text files or in Excel worksheets. (See “Z-matrix” on page 28 and “Cartesian Coordinates” on page 28 for more information.) Likewise, tables from text files or worksheets can be

copied into blank tables in Chem3D to create models. Text tables can use spaces or tabs between columns.

For a Cartesian table, there must be four columns (not including the Serial Number column) or five columns (if the Serial Number column is included.) The relative order of the the X-Y-Z columns must be preserved; otherwise column order is not important.

For a Z-Matrix table, there must be seven columns (not including Serial Number column) or eight columns (if the Serial Number column is included.) The column order must NOT be changed.

To copy a Cartesian or Z-Matrix table into Chem3D:

1. Select the table in the text or Excel file.
2. Use Ctrl+C to transfer to the clipboard.
3. Right-click in a blank table in Chem3D and select Paste.

Examples

Example 1: chloroethane Cartesian table (space character as separator)

```
C 0 -0.464725 0.336544 0.003670
C 0 0.458798 -0.874491 0.003670
Cl 0 0.504272 1.818951 0.003670
H 0 -1.116930 0.311844 0.927304
H 0 -1.122113 0.311648 -0.927304
H 0 -0.146866 -1.818951 0.003670
H 0 1.116883 -0.859095 0.923326
H 0 1.122113 -0.858973 -0.923295
```

Example 2: ethane Cartesian table (tab as separator)

```
C	-0.49560.57820.0037
C	0.4956-0.57820.0037
H	0.05521.55570.0037
H	-1.15170.52520.9233
H	-1.15690.5248-0.9233
H	-0.0552-1.55570.0037
H	1.1517-0.52520.9233
H	1.1569-0.5248-0.9233
```

Example 3: ethenol Z-Matrix table (tab as separator)

```
C
C	1	1.33
O	2	1.321	119.73
H	3	0.9782	1091	180
H	2	0.991	1193	180
H	1	0.9892	119.53	180
H	1	0.9882	1193	0
```

Changing an Atom to Another Element

To change an atom from one element to another:

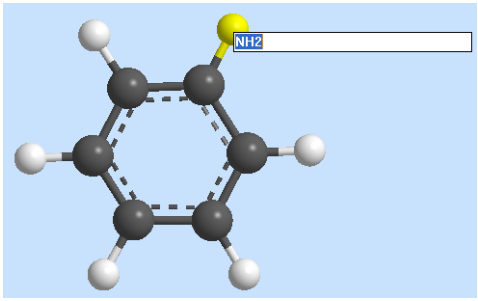
1. Click the Text tool.
2. Click the atom to change.

   A text box appears.
3. Type the symbol for the element you want (case-sensitive).
4. Press the Enter key.

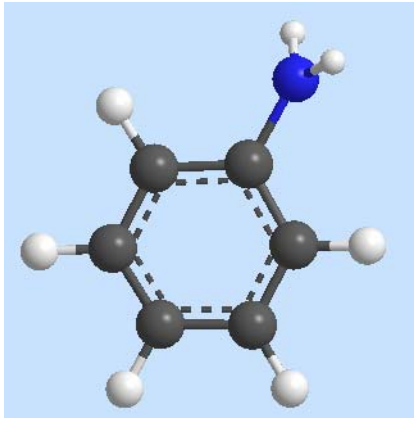
As long as the Text tool is selected, you can double-click other atoms to make the same change.

For example, to change benzene to pyridine:

1. Click the atom to replace and type NH2.



2. Press the Enter key.



Changing an Atom to Another Atom Type

To change a single atom:

1. Click the Text tool.
2. Click the atom to change.

   A text box appears.
3. Type the name of the atom type (case sensitive).
4. Press the Enter key.

To change more than one atom:

1. Use Shift+click to select the atoms to change.
2. Type the name of the atom type (case sensitive).
3. Press the Enter key.

For many atom types that change bond order, you must select all atoms attached to the bond so that the correct bond forms.

For example, to change ethane to ethene:

1. Select both carbons.
2. Type C Alkene.
3. Press the Enter key.

Changing Bonds

To change the bond order of a bond you can use the bond tools, commands, or the Text tool.

You can change the bond order in the following ways:

- One bond at a time.
- Several bonds at once.
- By changing the atoms types on the bond.

To change the bond order with the bond tool:

1. Select a bond tool (of a different order).
2. Drag from one atom to another to change.

To change the bond order using a command:

1. Select a bond.
2. From the Right-click menu, point to Set Bond Order, and choose a bond order.

To change the bond order by changing the atom type of the atoms on either end of the bond:

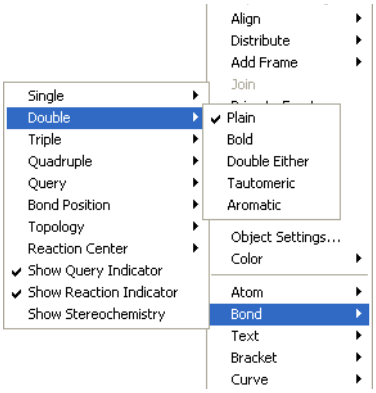
1. Click the Text tool.
2. Shift+click all the atoms that are attached to bonds whose order you want to change.

3. Type the atom type to which you want to change the selected atoms.
4. Press the Enter key.

   The bond orders of the bonds change to reflect the new atom types.

To change several bonds at once:

1. Open the ChemDraw panel and click in it to activate the ChemDraw control.
2. Choose either selection tool, Lasso or Marquee.
3. Click the first bond to be changed, then use Shift+Click to select the others.
4. Right-click in the selected area, and choose the bond type.



5. Click in the Chem3D window to complete the action.

Creating Bonds by Bond Proximate Addition

Atoms that are within a certain distance (the bond proximate distance) from one another can be automatically bonded.

Chem3D determines whether two atoms are proximate based on their Cartesian coordinates and the standard bond length measurement.

Pairs of atoms whose distance from each other is less than the standard bond length, plus a certain percentage, are considered proximate. The lower the percentage value, the closer the atoms have to be to the standard bond length to be considered proximate. Standard bond lengths are stored in the Bond Stretching Parameters table.

To set the percentage value:

1. From the File menu, choose Model Settings.

   The Chem 3D Model Settings dialog box appears.
2. Select the Model Build tab.
3. Use the Bond Proximate Addition% arrows to adjust the percentage added to the standard bond length when Chem3D assesses the proximity of atom pairs.

   You can adjust the value from 0 to 100%. If the value is zero, then two atoms are considered proximate only if the distance between them is no greater than the standard bond length of a bond connecting them. For example, if the value is 50, then two atoms are considered proximate if the distance between them is no greater than 50% more than the standard length of a bond connecting them.

To create bonds between proximate atoms:

1. Select the atoms that you want tested for bond proximity.
2. From the Right-click menu, point to Bond(s) and choose Proximate.

   If they are proximate, a bond is created.

Adding Fragments

A model can be composed of several fragments.

If you are using bond tools, begin building in a corner of the window.

If you are using the Text tool:

1. Click in an empty area of the window.

   A text box appears.
2. Type in the name of an element, atom type, or substructure.
3. Press the Enter key.

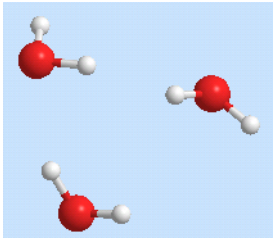
   The fragment appears.

For example, to add water molecules to a window containing a model of formaldehyde:

1. Click the Text tool.
2. Click in the approximate location you want a water molecule to appear.

   A text box appears.
3. Type H2O.
4. Press the Enter key.

   The fragment appears.
5. Double-click in a different location to add another H_2O molecule.



View Focus

As models become large, keeping track of the section you are working on becomes more difficult. With version 9.0.1, Chem3D adds the notion of "view focus", defined as the set of atoms that the user is interested in working on. By default, the view focus includes all of the atoms in the model.

To change the view focus to include only those atoms and bonds you are working on:

1. Select the fragment or set of atoms or bonds.
2. Click Set Focus to Selection on the View Focus submenu of the View menu.

Once you have set the view focus, the following things happen:

- When building with the bond tools, Chem3D will resize and reposition the view so that all of the atoms in the view focus are visible.
- As new atoms are added, they become part of the view focus.
- When rotating, or resizing the view manually, the rotation or resize will be centered around the view focus.

Setting Measurements

You can set the following measurements using the Measurements submenu of the Structure menu:

- Bond lengths
- Bond angles
- Dihedral angles
- Close contacts

NOTE: *When you choose Measurement from the Structure menu, the display of the Set Measurement option will vary, depending on what you have selected. The grayed-out option says Set Measurement; when you select a bond, it says Set Bond Length, etc.*

When you use the Clean Up Structure command, the bond length and bond angle values are overridden by the standard measurements from the Optimal column of the Measurement table. These optimal values are the standard measurements in the Bond Stretching and Angle Bending parameter tables. For all other measurements, performing a

Clean Up Structure or MM2 computation alters these values. To use values you set in these computations, you must apply a constraint.

Setting Bond Lengths

To set the length of a bond between two bonded atoms:

1. Select two adjacent atoms.
2. From the Structure menu, point to Measurement and choose Set Bond Length Measurement.

   The Measurements table appears, displaying distance between the two atoms. The Actual value is highlighted.
3. Edit the highlighted text.
4. Press the Enter key.

Setting Bond Angles

To set a bond angle:

1. Select three contiguous atoms for a bond angle.
2. From the Structure menu, point to Measurement and choose Set Bond Angle Measurement.

   The Measurements table appears, displaying the angle value. The Actual value is highlighted.
3. Edit the highlighted text.
4. Press the Enter key.

Setting Dihedral Angles

To set a dihedral angle:

1. Select four contiguous atoms.
2. From the Structure menu, point to Measurement and choose Set Dihedral Measurement.

   The Measurements table appears, displaying the angle value. The Actual value is highlighted.
3. Edit the highlighted text.
4. Press the Enter key.

Setting Non-Bonded Distances (Atom Pairs)

To set the distance between two non-bonded atoms (an atom pair):

1. Select two unbonded atoms.
2. From the Structure menu, point to Measurement and choose Set Distance Measurement.

   The Measurements table appears, displaying the distance. The Actual value is highlighted.
3. Edit the highlighted text.
4. Press the Enter key.

Atom Movement When Setting Measurements

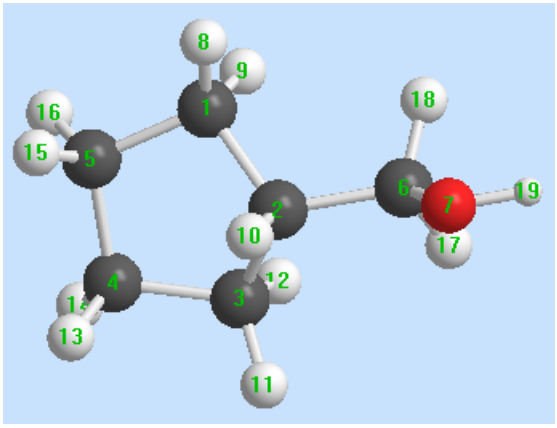
When you change the value of a measurement, the last atom selected moves. Chem3D determines which other atoms in the same fragment also move by repositioning the atoms that are attached to the moving atom and excluding the atoms that are attached to the other selected atoms.

If all of the atoms in a measurement are within a ring, the set of moving atoms is generated as follows:

- Only one selected end atom that describes the measurement moves while other atoms describing the measurement remain in the same position.
- If you are setting a bond length or the distance between two atoms, all atoms bonded to the non-moving selected atom do not move. This set of non-moving atoms is extended through all bonds. From among the remaining atoms, any atoms which are bonded to the moving atom move; this set of moving atoms is also extended through all bonds.

- If the Automatically Rectify check box in the Building control panel is selected, rectification atoms that are positioned relative to an atom that moves may also be repositioned.

For example, consider the following structure:



If you set the bond angle C(1)-C(2)-C(3) to 108 degrees, C(3) becomes the end moving atom. C(1) and C(2) remain stationary. H(11) and H(12) move because they are not part of the ring but are bonded to the moving atom. If the Automatically Rectify check box is selected, H(10) may move because it is a rectification atom and is positioned relative to C(3).

Setting Constraints

You can override the standard measurements which Chem3D uses to position atoms by setting constraints. Constraints can be used to set an optimal value for a particular bond length, bond angle, dihedral angle, or non-bonded distance, which is then applied instead of the standard measurement when you use Clean Up Structure or perform a Docking, Overlay, or MM2 computation.

To set constraints:

- Enter a new value for the constraint in the Optimal field of the Measurements table.

In the case of dihedral angles and non-bonded distances, a constraint will have the effect of keeping that measurement constant (or nearly so) while the remainder of the model is changed by the computation. The constraint doesn't remove the atoms from a computation.

Setting Charges

Atoms are assigned a formal charge based on the atom type parameter for that atom and its bonding. You can display the charge by pointing to the atom.

To set the formal charge of an atom:

1. Click the Text tool.
2. Select the atom or atoms to change.
3. Type + or - followed by the number of the formal charge.
4. Press the Enter key.

To set the formal charge of an atom in a molecular fragment as you build you can add the charge after the element in the text as you build.

To add the charge:

1. Type PhO- into a text box with no atoms selected.
2. Press the Enter key.

   The phenoxide ion molecule appears.

To remove the formal charge from an atom:

1. Click the Text tool.
2. Select the atom or atoms whose formal charge you want to remove.
3. Type +0.
4. Press the Enter key.

Setting Serial Numbers

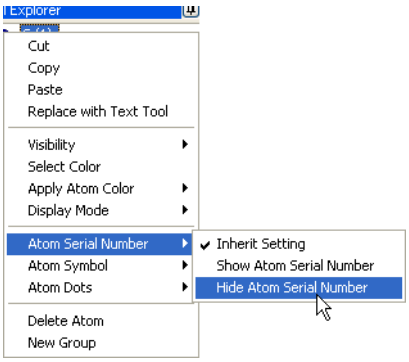
Atoms are assigned serial numbers when they are created. You can view the serial numbers in the following ways:

- Point to the atom to display the pop-up information.
- From the Model Display submenu of the View menu, choose Show Serial Numbers.
- In the Chem 3D Model Settings dialog box, choose the Atom Labels tab, and then check the Show Serial Numbers checkbox.
- Click the Serial Number toggle on the Model Display Toolbar.

Serial numbers are initially assigned based on the order in which you add atoms to your model.

To change the serial number of an atom:

1. If you are using the Model Explorer, select the atoms you want to re-number, and select Hide Atom Serial Number from the Atom Serial Numbers submenu of the context menu.



NOTE: *The Model Explorer cannot update its numbering to match the changes you are making on the model when Serial Numbers are displayed. If you forget this step, you will see different numbers on the tree control and the model. If this happens, simply hide the serial numbers momentarily and redisplay them.*

2. Click the Text tool.
3. Click the atom to reserialize.

   A text box appears.
4. Type the serial number.
5. Press the Enter key.

If the serial numbers of any unselected atoms conflict with the new serial numbers, then those unselected atoms are renumbered also.

To reserialize another atom with the next sequential number:

- Double-click the next atom you want to reserialize.

To reserialize several atoms at once:

1. Click the Text tool.
2. Hold down Shift and select several atoms.
3. Type the starting serial number.
4. Press the Enter key.

Normally, the selected atoms are reserialized in the order of their current serial numbers. However, the first four atoms selected are reserialized in the order you selected them.

Changing Stereochemistry

You can alter the stereochemistry of your model by inversion or reflection.

Inversion

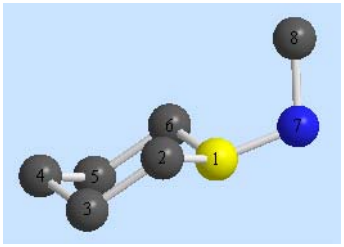
The Invert command performs an inversion symmetry operation about a selected chiral atom.

To perform an inversion:

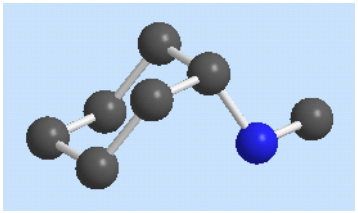
1. Select the atom.
2. From the Structure menu, choose Invert.

   The Invert command only repositions side chains extending from an atom.

For example, if you choose Invert for the structure below when C(1) is selected:



The following structure appears.



To invert several dihedral angles (such as all of the dihedral angles in a ring) simultaneously:

1. Select the dihedral angles to invert.
2. From the Structure menu, choose Invert stereochemistry.

   All of the dihedral angles that make up the ring are negated. Atoms positioned axial to the ring are repositioned equatorial. Atoms positioned equatorial to the ring are repositioned axial.

Reflection

use the Reflect command to perform reflections on your model through any of the specified planes.

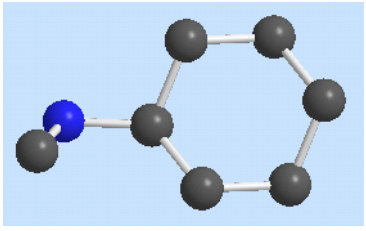
When you choose the Reflect commands certain Cartesian coordinates of each of the atoms are negated. When you choose Reflect Through Y-Z Plane, all of the X coordinates are negated. You can choose Reflect Through X-Z Plane to negate all of the Y coordinates. Likewise, you can choose Reflect Through X-Y Plane to negate all of the Z coordinates. You can choose Invert through Origin to negate all of the Cartesian coordinates of the model.

If the model contains any chiral centers, each of these commands change the model into its enantiomer. If this is done, all of the Pro-R positioned atoms become Pro-S and all of the Pro-S positioned atoms become Pro-R. All dihedral angles used to position atoms are negated.

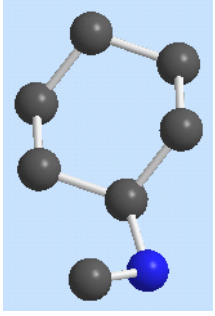
NOTE: *Pro-R and Pro-S within Chem3D are not equivalent to the specifications R and S used in standard chemistry terminology.*

For example, for the structure below, when any atom is selected:

- From the Structure menu, point to Reflect Model and choose Through X-Z Plane.



Chem3D produces the following structure (an enantiomer):



Refining a Model

After building a 3D structure, you may need to clean it up. For example, if your model was built without automatic rectification, atom type assignment, or standard measurements, you can apply these as a refinement.

Rectifying Atoms

To rectify the selected atoms in your model:

- From the Structure menu, choose Rectify.

  Hydrogen atoms are added and deleted so that each selected atom is bonded to the correct number of atoms as specified by the geometry for its atom type. This command also assigns atom types before rectification.

  The atom types of the selected atoms are changed so that they are consistent with the bound-to orders and bound-to types of adjacent atoms.

Cleaning Up a Model

Normally, Chem3D creates approximately correct structures. However, it is possible to create unrealistic structures, especially when you build strained ring systems. To correct unrealistic bond lengths and bond angles use the Clean Up Structure command.

To clean up the selected atoms in a model:

- From the Structure menu, choose Clean Up .

  The selected atoms are repositioned to reduce errors in bond lengths and bond angles. Planar atoms are flattened and dihedral angles around double bonds are rotated to 0 or 180 degrees.

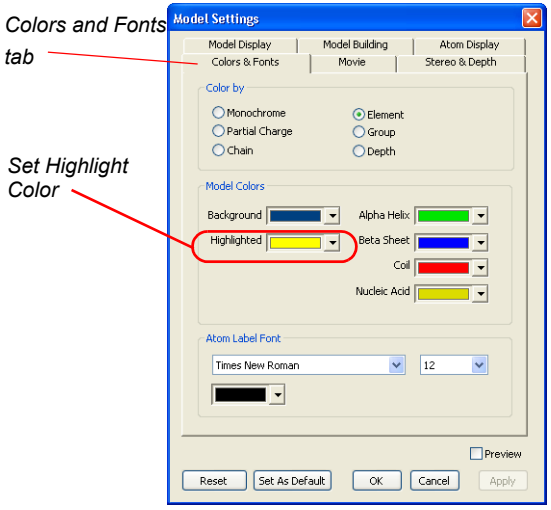
Chapter 5: Manipulating Models

Overview

Chem3D provides tools to manipulate the models you create. You can show or hide atoms and select groups to make them easier to manipulate. Molecules can be rotated, aligned, and resized.

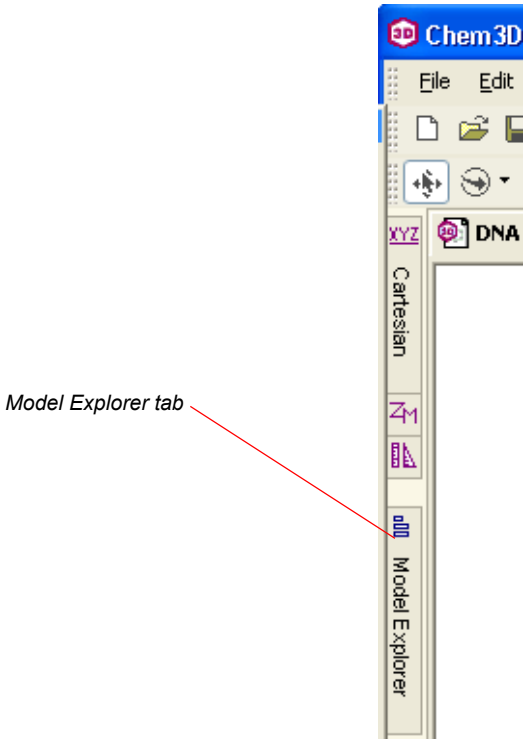
Selecting

Most operations require that the atoms and bonds that are operated on be selected. Selected atoms and bonds are highlighted in the model display. You can change the default highlight color in the Model Settings dialog box.



Selecting Single Atoms and Bonds

You can select atoms and bonds in the model window or by using the Model Explorer. If the Model Explorer is not active, open it from the View menu.



To select an atom using the Model Explorer:

1. Open the Model Explorer.
2. Select the atom in the Explorer.

   The atom is selected in the model. Any previously selected atoms or bonds are deselected.

To select an atom or bond in the display window:

1. Click the Select tool .
2. Click the atom or bond.

   Any previously selected atoms and bonds are deselected. When you click a bond, both atoms on the bond are selected.

Selecting Multiple Atoms and Bonds

To select multiple individual atoms and bonds, do one of the following:

- Shift+click atoms or bonds in the display window to select them.
- Ctrl+click atoms in the Model Explorer to select them.
- Shift+click atoms in the Model Explorer to select all atoms between (and including) the two selected.

> ***NOTE:*** *Selecting two adjacent atoms will also select the bond between them.*

To quickly select all atoms and bonds in a model:

- From the Edit menu, choose Select All.

> ***NOTE:*** *If the last action performed was typing in a text box, all of its text is selected instead of the atoms in the model.*

Deselecting Atoms and Bonds

When you deselect an atom, you deselect all adjacent bonds. When you deselect a bond, you deselect the atoms on either end if they are not also connected to another selected bond.

To deselect a selected atom or bond, do one of the following:

- Shift+click the atoms or bonds in the display window.
- Ctrl+click the atom in the Model Explorer.

If Automatically Rectify is on when you deselect an atom, adjacent rectification atoms and lone pairs are also deselected.

> ***NOTE:*** *A rectification atom is an atom bonded to only one other atom and whose atom type is the rectification type for that atom.*

To deselect all atoms and bonds:

- Click in an empty area of the Model window.

With the Model Explorer, you can use different selection highlight colors for different fragments or groups. To change the highlight color in the Model Explorer:

- Right-click at any level and choose Select Color.

See "Working With the Model Explorer" on page 111 for information on other functions of the Model Explorer.

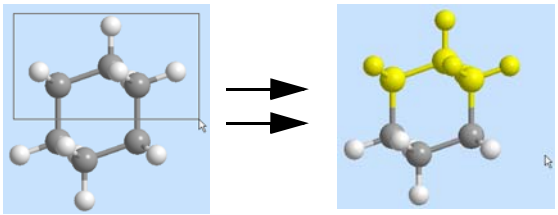
Selecting Groups of Atoms and Bonds

You can define groups of atoms (and fragments or large models) and use the Model Explorer to select the entire group. You can also select groups of atoms without defining them as a group with the selection rectangle.

Using the Selection Rectangle

To select several atoms and bonds using the Selection Rectangle:

- Drag diagonally across the atoms you want to select.



Any atoms that fall at least partially within the Selection Rectangle are selected when you release the mouse button. A bond is selected only if both atoms connected by the bond are also selected.

To keep previously selected atoms selected:

- Hold down the Shift key while you make another selection.

  If you hold down the Shift key and all of the atoms within the Selection Rectangle are already selected, then these atoms are deselected.

Defining Groups

You can define a portion of your model as a group. This provides a way to easily select and to highlight part of a model (such as the active site of a protein) for visual effect.

To define a group:

1. Select the atoms and bonds you want in the group. Using the select tool, select the first atom then use Shift+click to select the other atoms and bonds.
2. While still pointing at one of the selected atoms, right-click and choose New Group from the Context-Sensitive menu.

If the groups in your model are substructures defined in the Substructures table (substructures.xml), you can assign standard colors to them.

To assign (or change) a color:

1. From the View menu, point to Parameter tables and select Substructures.
2. Double click in a cell in the Color field.

   The Color dialog box appears.
3. Select a color and click OK.
4. Close and Save the Substructures table.

Once colors are assigned in the Substructures table, you can use them to apply color by group:

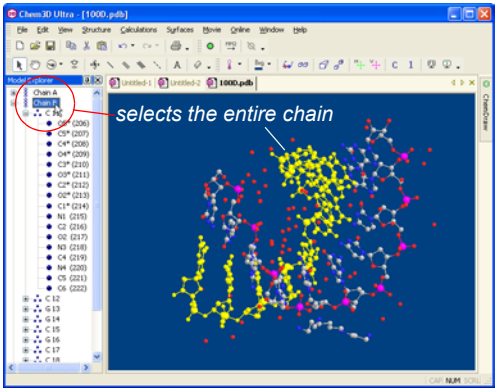
1. From the File menu, choose Model Settings.
2. Select the Model Display control panel.
3. Select the Group radio button in the Color by section.

   Each atom in your model appears in the color specified for its group.

NOTE: *Color by Group is only displayed when Ribbon or Cartoon display mode is selected.*

Selecting a Group or Fragment

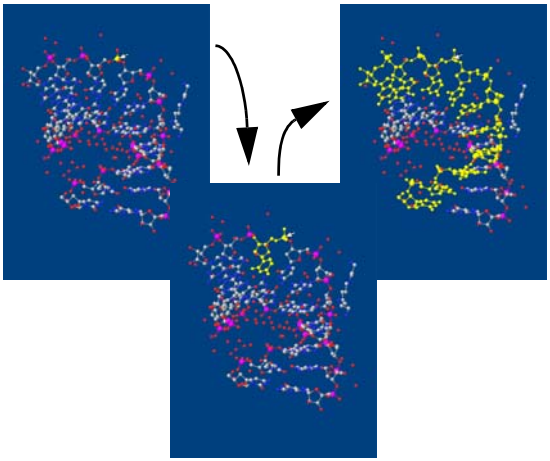
There are several ways to select a group or fragment. The simplest is to use the Model Explorer, and select the fragment.



You may also select a single atom or bond and use the Select Fragment command on the Edit menu.

NOTE: *If you want to select more than one fragment, you must use the Model Explorer.*

New in Chem3D version 9.0.1 is double-click selection. After you have selected a single atom or bond, each successive double-click will select the next higher level of hierarchy.



Selecting Atoms or Groups by Distance

You can select atoms or groups based on the distance or radius from a selected atom or group of objects. This feature is useful, among other things, for highlighting the binding site of a protein.

To select atoms or groups by distance:

1. Use the Model Explorer to select an atom or fragment.
2. Right-click the selected object. From the context menu point to Select and click the
3. appropriate option:

Option	Result
Select Atoms within Distance of Selection	Selects all atoms lying within the specified distance from any part of the current selection.
Select Groups within Distance of Selection	Selects all groups that contain one or more atoms lying within the specified distance from any part of the current selection.
Select Atoms within Radius of Selection Centroid	Selects all atoms lying within the specified distance of the centroid of the current selection.
Select Groups within Radius of Selection Centroid	Selects all groups that contain one or more atoms lying within the specified distance of the centroid of the current selection.

NOTE: *1. Atoms or groups already selected are not included.*
2. The current selection will be un-selected unless multiple selection is used. Hold the shift key down to specify multiple selection.

Showing and Hiding Atoms

You may want to view your models with different atoms visible or not visible. You can temporarily hide atoms using the Model Explorer. To hide atoms or groups:

- Right-click at any level, point to Visibility and click Hide... (Atom Group, etc.).

  Hidden atoms or groups are displayed in parentheses in the tree control.

By default, all levels in the hierarchy are set to inherit the settings of the level above, but you can reset the default to hide a group but show individual atoms in it. To show an atom belonging to a hidden group:

- Right-click on the atom in the tree control, point to Visibility and choose Show.

Showing Hs and Lps

To show all hydrogen atoms and lone pairs in the model:

- From the Model Display submenu of the View menu, choose Show H's and Lp's.

  A check mark appears beside the command, indicating that it has been selected.

When Show Hs and Lps is not selected, hydrogen atoms and lone pairs are automatically hidden.

Showing All Atoms

If you are working with a large model, it may be difficult to keep track of everything you have hidden. To show all atoms or groups that are hidden:

1. Select a level in the tree control above the hidden atoms or groups, or Shift+click to select the entire model.
2. From the Right-click menu point to Select and click Select All Children.
3. Right-click again, point to Show... and choose Inherit Setting.

Moving Atoms or Models

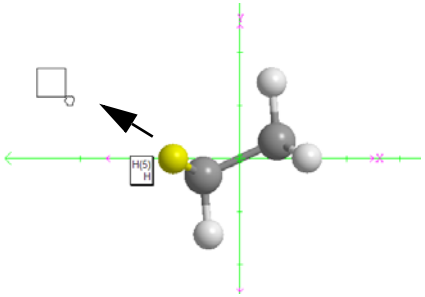
Use the Move Objects tool to move atoms and other objects to different locations. If the atom, group of atoms, bond, or group of bonds that you want to move are already selected, then all of the selected atoms move. Using the Move Objects tool changes the view relative to the model coordinates.

The following examples use the visualization axes to demonstrate the difference between different types of moving. To move an atom to a different location on the X-Y plane:

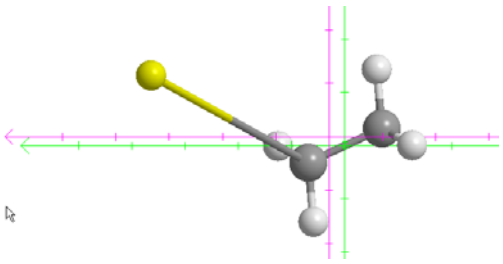
1. Click both the Model Axis and View Axis tools to visualize the axes.

   NOTE: *The axes will only appear if there is a model in the window.*

2. Drag with the single bond tool to create a model of ethane.
3. Point to an atom using the Move Objects Tool.
4. Drag the atom to a new location.



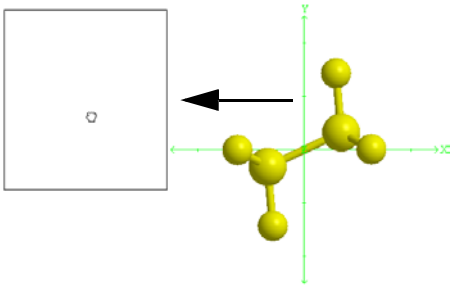
Dragging moves atoms parallel to the X-Y plane, changing only their X- and Y-coordinates.



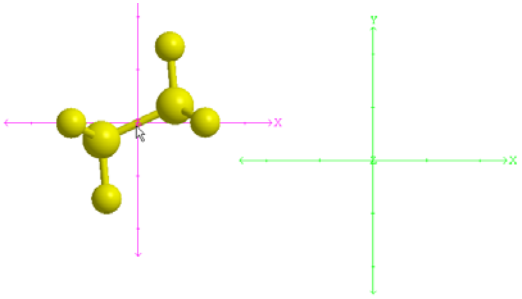
If Automatically Rectify is on, then the unselected rectification atoms that are adjacent to selected atoms move with the selected atoms.

To move a model:

1. With the Move Objects tool, drag across the model select it.
2. Drag the model to the new location.

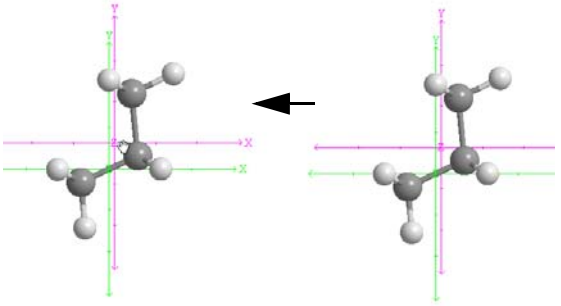


Note that the View axis has moved relative to the model coordinates.



Moving Models with the Translate Tool

Use the Translate tool to move a model in the view window. When you use the Translate tool, you move both the focus view and the model coordinates along with the model. Thus, the model's position does not change relative to the origin.



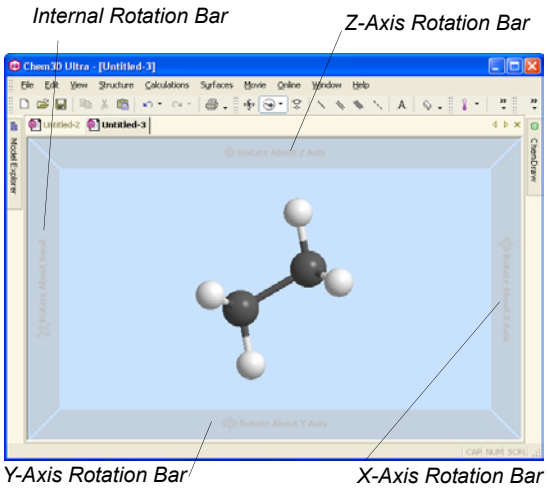
Rotating Models

Chem3D allows you to freely rotate the model around axes. When you select the Trackball tool, four pop-up rotation bars are displayed on the periphery of the model window. You can use these rotation bars to view your model from different angles by rotating around different axes. You can also open the Rotate dialog box where you can use the rotate dial or type the number of degrees to rotate.

To display the Rotation bars:

- Select the Trackball tool from the Building toolbar.

When you mouse over an edge of the model window, the Rotation bars appear on the edges of the Model window.



X- Y- or Z-Axis Rotations

To perform a rotation about the X-, Y-, or Z-axis:

1. Point to the appropriate Rotation bar.
2. Drag the pointer along the Rotation bar.

   The number of degrees of rotation appears in the Status bar.

Rotating Fragments

If more than one model (fragment) is in the model window, you can rotate a single fragment or rotate all fragments in the model window.

To rotate only one fragment:

1. Select an atom in the fragment you want to rotate.
2. Drag a rotation bar.

To rotate all fragments, do **one** of the following:

- With an atom selected, Shift+drag a Rotation bar.
- With no atoms selected, drag a rotation bar.

Trackball Tool

Use the Trackball tool to freely rotate a model.

- Starting anywhere in the model window, drag the pointer in any direction

  The Status bar displays the X and Y axis rotation.

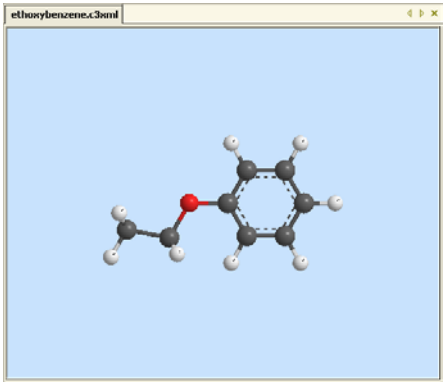
Internal Rotations

Internal rotations alter a dihedral angle and create another conformation of your model. You can rotate an internal angle using the Internal Rotation bar.

To perform internal rotations in a model, you must select at least two atoms or one bond.

Internal rotation is typically specified by a bond. The fragment at one end of the bond is stationary while the fragment attached to the other end rotates. The order in which you select the atoms determines which fragment rotates. (See the following examples.)

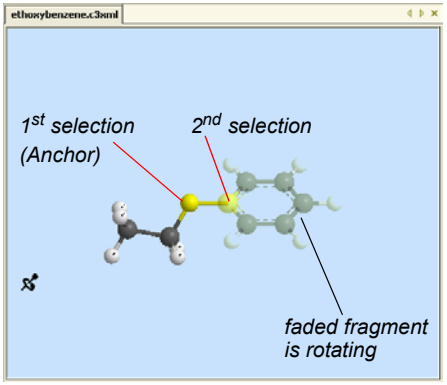
For example, consider ethoxybenzene (phenetole):



To perform a rotation about the C-O bond where the phenyl group moves:

1. Select the Trackball tool.
2. Hold down the S key, and select the O atom.

3. Hold down the Shift and S keys, and select the C1 atom.
4. Drag the pointer along the Internal Rotation bar.



To perform a rotation about the C-O bond where the ethyl group moves:

1. Reverse the order of selection: first select C1, then O.

   TIP: *To deselect the atoms, hold down the S key and click anywhere in the model window.*

2. Drag the pointer along the Internal Rotation bar.

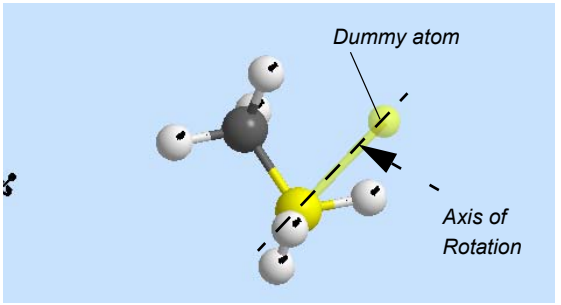
Rotating Around a Bond

To rotate the model around a specific bond:

1. Select a bond.
2. Hold down the Shift key and drag the pointer along the Internal Rotation bar.

Rotating Around a Specific Axis

You can rotate your model around an axis you specify by selecting any two atoms in your model. You can add dummy atoms as fragments to specify an axis around which to rotate.



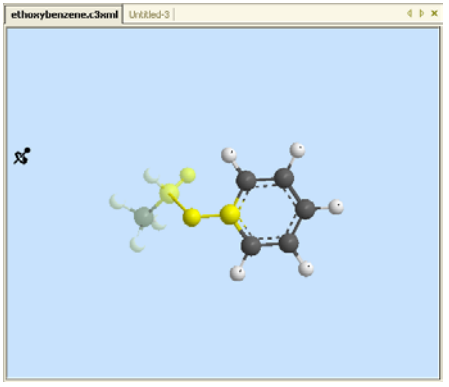
To rotate the model around an axis:

1. Select any two atoms.
2. Drag the pointer along the Internal Rotation bar.

Rotating a Dihedral Angle

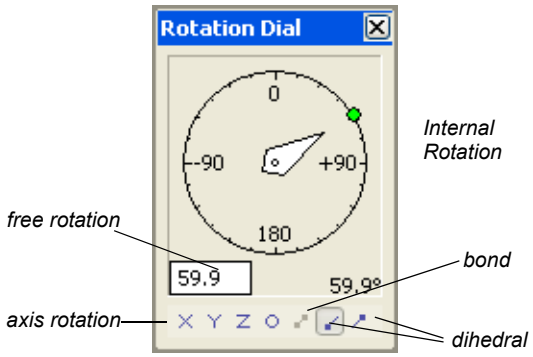
You can select a specific dihedral angle to rotate. To rotate a dihedral:

1. Select four atoms that define the dihedral.
2. Drag the pointer along the Internal Rotation bar.



Using the Rotation Dial

The Rotation Dial offers a quick method of rotating a model or dihedral a chosen number of degrees with reasonable accuracy. For more precision, you can enter exact numbers into the degree display box. The Internal Rotation icons are only available when atoms or bonds have been selected in the model.



Changing Orientation

Chem3D allows you to change the orientation of your model along a specific axis. However your model moves, the origin of the model (0, 0, 0) does not change, and is always located in the center of the model window. To change the origin, see "Centering a Selection" on page 100.

Aligning to an Axis

To position your model parallel to either the X-, Y-, or Z-axis:

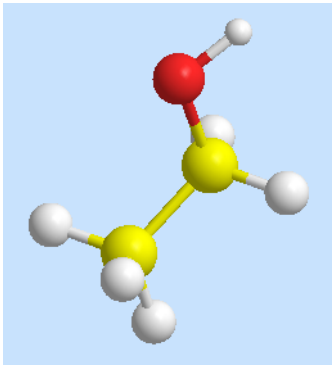
1. Select two atoms only.
2. From the View menu, point to View Position, and then click Align View (choose an axis) With Selection.

   The model rotates so that the two atoms you select are parallel to the appropriate axis.

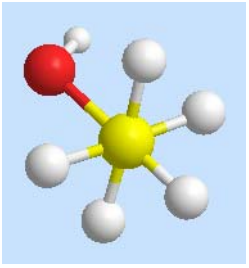
> ***NOTE:*** *This changes the view, not the coordinates of the molecule. To change the model coordinates, use the* Model Position *submenu of the* Structure *menu.*

For example, to see an end-on view of ethanol:

1. Click the Select tool.
2. Shift+click C(1) and C(2).



3. From the View menu, point to View Position, and then click Align View Z Axis With Selection.



Aligning to a Plane

You can align a model to a plane when you select three or more atoms. When you select three atoms, those atoms define a unique plane. If you select more than three atoms, a plane is computed that minimizes the average distance between the selected atoms and the plane.

To position a plane in your model parallel to a plane of the Cartesian Coordinate system:

1. Select three or more atoms.
2. From the View menu, point to View Position, and then click Align View (choose a plane) With Selection.

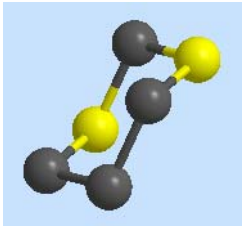
   The entire model rotates so that the computed plane is parallel to the X-Y, Y-Z, or X-Z plane. The center of the model remains in the center of the window.

To move three atoms to a plane and two of the atoms onto an axis:

1. Select the two atoms.
2. From the View menu, point to View Position, and then click Align View (choose an axis) With Selection.
3. Shift+click the third atom.
4. From the View menu, point to View Position, and then click Align View (choose a plane) With Selection.

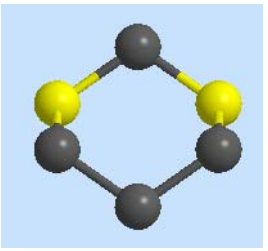
For example, to move a cyclohexane chair so that three alternating atoms are on the X-Y Plane:

1. Select two non-adjacent carbon atoms in the ring.



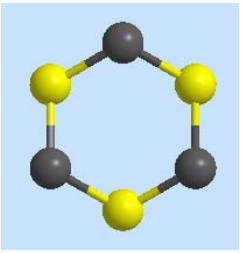
2. From the View menu, point to View Position, and then click Align View X Axis With Selection.

   The model moves to the position shown below.



3. Select the third carbon atom such that no two selected atoms in the ring are adjacent.
4. From the View menu, point to View Position, and then click Align View X-Y Plane With Selection.

   The model moves to the position shown below.



Resizing Models

Chem3D provides the following ways to resize your model:

- Resizing Windows
- "Scaling a Model"

Centering a Selection

When resizing a model, or before doing computations, it is often useful to center the model. Chem3D allows you to select an atom (or atoms) to determine the center, or performs the calculation on the entire model.

To center your model based on a particular selection:

1. Select one or more atoms. (optional)
2. Choose Center Model from the Model Position submenu of the Structure menu.

This command places the centroid of the selected atoms at the coordinate origin. Chem3D calculates the centroid of the selected atoms by averaging their X, Y, and Z coordinates. If you do not select any atoms, the command operates on the entire model.

NOTE: *This command affects all frames of your model, not just the active frame.*

Using the Zoom Control

You can reduce or enlarge a model using the Zoom tool.

NOTE: The Zoom tool lets you resize the model by dragging.*This changes the view, not the coordinates of the molecule.*

Scaling a Model

You can scale a model to fit a window. If you have created a movie of the model, you have a choice of scaling individual frames or the whole movie.

To scale a model to the window size, do one of the following:

- From the View menu, point to View Position and click Fit To Window.
- From the View menu, point to View Position and choose Fit All Frames To Window to scale an entire movie.

The Model To Window command operates only on the active frame of a movie. To scale more than one frame, you must repeat the command for each frame you want to scale.

NOTE: *The Fit command only affect the scale of the model. Atomic radii and interatomic distances do not change.*

Changing the Z-matrix

The relative position of each atom in your model is determined by a set of internal coordinates known as a Z-matrix. The internal coordinates for any particular atom consist of measurements (bond lengths, bond angles, and dihedral angles) between it and other atoms. All but three of the atoms in your structure (the first three atoms in the Z-matrix which describes your model) are positioned in terms of three previously positioned atoms.

To view the current Z-matrix of a model:

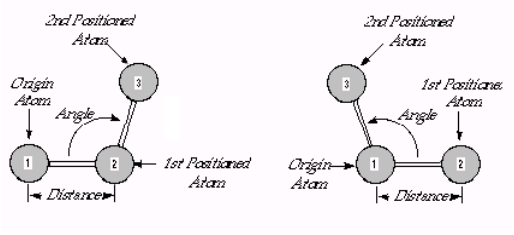
- From the View menu choose Z-Matrix Table.

The First Three Atoms in a Z-matrix

The first three atoms in a Z-matrix are defined as follows:

- **Origin atom**—The first atom in a Z-matrix. All other atoms in the model are positioned (either directly or indirectly) in terms of this atom.
- **First Positioned atom**—Positioned only in terms of the Origin atom. Its position is specified by a distance from the Origin atom. Usually, the First Positioned atom is bonded to the Origin atom.

- **Second Positioned atom**—Positioned in terms of the Origin atom and the First Positioned atom. There are two possible ways to position the Second Positioned atom, as described in the following example.



In the left example, the Second Positioned atom is a specified distance from the First Positioned atom. In addition, the placement of the Second Positioned atom is specified by the angle between the Origin atom, the First Positioned atom, and the Second Positioned atom.

In the right example, the Second Positioned atom is a specified distance from the Origin atom. In addition, the placement of the Second Positioned atom is specified by the angle between the First Positioned atom, the Origin atom, and the Second Positioned atom.

Atoms Positioned by Three Other Atoms

In the following set of illustrations, each atom D is positioned relative to three previously positioned atoms C, B, and A. Three measurements are needed to position D: a distance, and two angles.

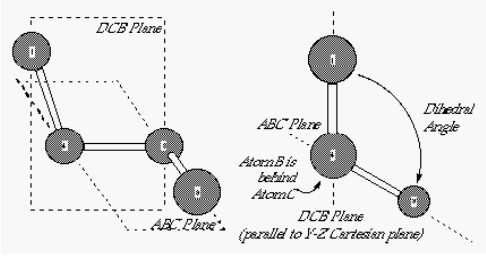
Atom C is the Distance-Defining atom; D is placed a specified distance from C. Atom B is the First Angle-Defining atom; D, C, and B describe an angle.

Atom A is the Second Angle-Defining atom. It is used to position D in one of two ways:

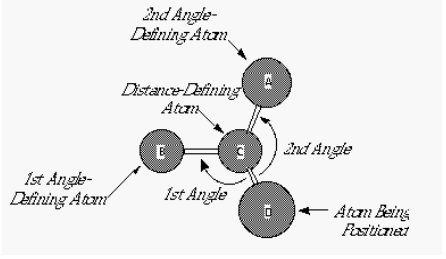
- By a dihedral angle A-B-C-D
- By a second angle A-C-D.

In the left example, atom D is positioned in terms of a dihedral angle, thus the second angle is the dihedral angle described by A-B-C-D. This dihedral angle is the angle between the two planes defined by D-C-B and A-B-C.

In the right example, if you view down the C-B bond, then the dihedral angle appears as the angle formed by D-C-A. A clockwise rotation from atom D to atom A when C is in front of B indicates a positive dihedral angle.



When D is positioned using two angles, there are two possible positions in space about C for D to occupy: a Pro-R position and a Pro-S position.

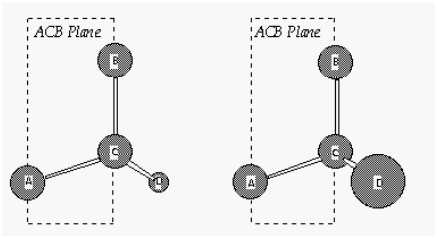


NOTE: *The terms Pro-R and Pro-S used in Chem3D to position atoms bear no relation to the Cahn-Ingold-Prelog R/S specification of the absolute stereochemical configuration of a chiral atom. Pro-R and Pro-S refer only to the positioning of D and do not imply any stereochemistry for C. C may be chiral, or achiral.*

The most convenient way to visualize how the Pro-R/Pro-S terms are used in Chem3D to position D is described in the following examples:

To position Atom D in Pro-S Orientation (left) and Pro-R Orientation (right):

1. Orient the Distance-Defining atom, C, the First Angle-Defining atom, B, and the Second Angle-Defining atom, A, such that the plane which they define is parallel to the X-Y plane.
2. Orient the First Angle-Defining atom, B, to be directly above the Distance-Defining atom, C, such that the bond joining B and C is parallel to the Y-axis, and the Second Angle-Defining atom, A, is somewhere to the left of C.



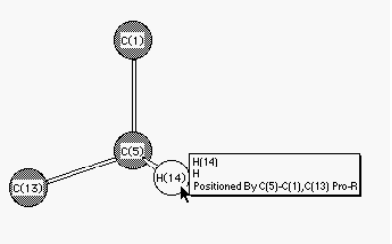
In this orientation, D is somewhere in front of the plane defined by A, B and C if positioned Pro-R, and somewhere behind the plane defined by A, B and C if positioned Pro-S.

When you point to or click an atom, the information box which appears can contain information about how the atom is positioned.

Positioning Example

If H(14) is positioned by C(5)-C(1), C(13) Pro-R, then the position of H(14) is a specified distance from C(5) as described by the H(14)-C(5) bond length. Two bond angles, H(14)-C(5)-C(1), and H(14)-C(5)-C(13), are also used to position the atom.

Because H(14) is positioned by two bond angles, there are two possible positions in space about C(5) for H(14) to occupy; the Pro-R designation determines which of the two positions is used.



If an atom is positioned by a dihedral angle, the three atoms listed in the information about an atom would all be connected by dashes, such as C(6)-C(3)-C(1), and there would be no Pro-R or Pro-S designation.

The commands in the Set Z-Matrix submenu allow you to change the Z-matrix for your model using the concepts described previously.

Because current measurements are retained when you choose any of the commands in the Set Z-Matrix submenu, no visible changes in the model window occur.

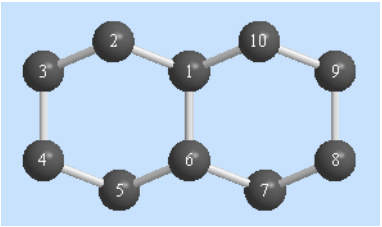
Positioning by Bond Angles

To position an atom relative to three previously positioned atoms using a bond distance and two bond angles:

1. With the Select tool, click the second angle-defining atom.
2. Shift-click the first angle-defining atom.
3. Shift-click the distance-defining atom.
4. Shift-click the atom to position.

   You should now have four atoms selected, with the atom to be positioned selected last.
5. From the Structure menu, point to Set Z-Matrix, and then choose Position by Bond Angles.

For example, consider the following structure:



To position atom C(7) by two bond angles, select atoms in the following order: C(5), C(1), C(6), C(7), then choose Position by Bond Angles.

Positioning by Dihedral Angle

To position an atom relative to three previously positioned atoms using a bond distance, a bond angle, and a dihedral angle:

1. With the Select tool, click the dihedral-angle defining atom.
2. Shift-click the first angle-defining atom.
3. Shift-click the distance-defining atom.
4. Shift-click the atom to position.

   You should now have four atoms selected, with the atom to be positioned selected last.
5. From the Structure menu, point to Set Z-Matrix, and then choose Position by Dihedral.

For example, using the previous illustration, choose atoms in the following order: C(7), C(6), C(1), C(10) to position C(10) by a dihedral angle in a ring. Then choose Position by Dihedral.

Setting Origin Atoms

To specify the origin atoms of the Z-matrix for a model:

1. With the Select tool, click the first one, two, or three atoms to start the Z-matrix.
2. From the Structure menu, point to Set Z-Matrix, and then choose Set Origin Atom or Set Origin Atoms.

   The selected atoms become the origin atoms for the Z-matrix and all other atoms are positioned relative to the new origin atoms. Because current measurements are retained, no visible changes to the model occur.

Chapter 6: Inspecting Models

Model Data

You can view information about an active model as a pop-up or in measurement windows.

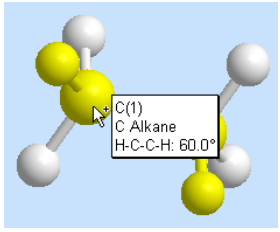
Pop-up Information

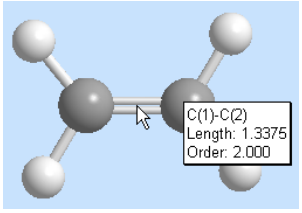
You can display information about atoms and bonds by pointing to them so that pop-up information appears. You specify what information appears by using the Pop-up Info tab of the Preferences dialog box.

You can display the following information about an atom:

- Cartesian coordinates
- Atom type
- Internal coordinates (Z-matrix)
- Measurements
- Bond Length
- Bond Order
- Partial Charge

Examples of pop-up information are shown below:





NOTE: *Precise bond orders for delocalized pi systems are displayed if the MM2 Force Field has been computed.*

The information about an atom or bond always begins with the name of that object, such as C(12) for an atom or O(5)-P(3) for a bond.

To set what pop-up information appears:

If you want to display ...	Then Select...
The three numerical values indicating the atom's position along the X, Y, and Z axes	Cartesian Coordinates.
the atom type corresponding to the first column of a record in the Atom Types table	Atom Type.
a list of the atoms used to position the atom	Z-matrix. *NOTE: The Z-matrix definition includes whether the second angle used to position the selected atom is a dihedral angle or a second bond angle.* *If atoms other than the one at which you are pointing are selected, the*

If you want to display ...	Then Select...
	measurement formed by all the selected atoms appears.
information relative to other selected atoms, such as the distance between two atoms, the angle formed by three atoms, or the dihedral angle formed by four atoms.	Measurements
the distance between the atoms attached by a bond in angstroms	Bond Length.
the bond orders calculated by Minimize Energy, Steric Energy, or Molecular Dynamics	Bond Order. Bond orders are usually 1.000, 1.500, 2.000, or 3.000 depending on whether the bond is a single, delocalized, double, or triple bond. Computed bond orders can be fractional.
the partial charge according to the currently selected calculation	Partial Charge. See "Displaying Molecular Surfaces" on page 64 for information on how to select a calculation.

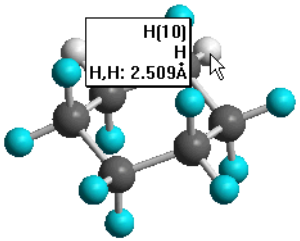
Non-Bonded Distances

To display non-bonded atoms measurements:

- Select two non-bonded atoms and point to one of them.

The interatomic non-bonded distance appears in the last line of the pop-up window.

For example, in the cyclohexane model below, when you select two non-bonded atoms and point to one of them, the interatomic non-bonded distance appears in the last line of the pop-up window.



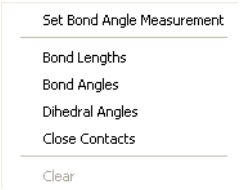
Measurement Table

Another way to view information about your model is to activate the Measurement Table. This table can display internal measurements between atoms in your model in various ways.

To display internal measurements:

1. From the View menu, click Measurement Table.

   A blank table appears in the Tables window.
2. From the Structure menu, point to Measurements and select a measurement to display.



The measurement values appear in the table.

You can display several measurements sequentially in the table. The following table shows the bond lengths and angles for Ethene.

Measurement

		Atoms	Actual	Optimal
1		H(5)-C(2)	1.1000	1.1000
2	bond lengths	C(2)-H(6)	1.1000	1.1000
3	bond lengths	H(3)-C(1)	1.1000	1.1000
4	bond lengths	C(1)-C(2)	1.3370	1.3370
5	bond lengths	C(1)-H(4)	1.1000	1.1000
6		H(5)-C(2)-H(6)	118.9990	119.0000
7	bond angles	H(5)-C(2)-C(1)	120.4999	120.5000
8	bond angles	H(6)-C(2)-C(1)	120.4987	120.5000
9	bond angles	H(3)-C(1)-C(2)	120.4999	120.5000
10	bond angles	H(3)-C(1)-H(4)	118.9990	119.0000
11		C(2)-C(1)-H(4)	120.4987	120.5000

Editing Measurements

If you select a measurement in the Measurements table, the corresponding atoms are selected in the model window. If you select atoms in your model, any corresponding measurements are selected.

To change the value of a measurement:

1. Select the text in the Actual column.
2. Type a new measurement value in the selected cell.
3. Press the Enter key

   The model reflects the new measurement.

When atoms are deleted, any measurements that refer to them are removed from the Measurements table.

Optimal Measurements

Optimal values are used instead of the corresponding standard measurements when a measurement is required in an operation such as Clean Up Structure. Optimal measurements are only used when the Measurements table is visible.

When the Measurements table is not visible, the standard measurements are taken from the parameter tables.

To specify optimal values for particular measurements, edit the value in the Optimal column.

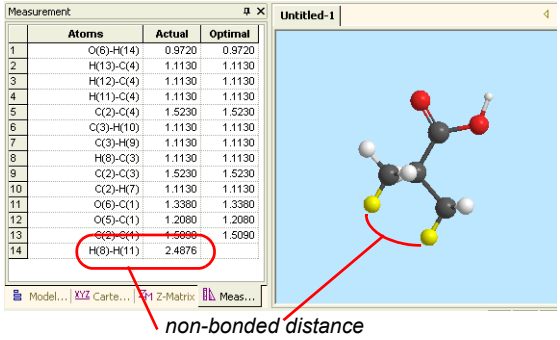
Chem3D also uses the optimal values with the Dock command. When you choose Dock from the Structure menu, Chem3D reconciles the actual distance between atoms in two fragments to their optimal distances by rigidly moving one fragment relative to the other.

Non-Bonded Distances in Tables

To display non-bonded atom measurements:

1. Select the atoms.
2. From the Structure menu, point to Measurements and choose Set Distance Measurement.

   The measurement between the selected atoms is added to the table.



Showing the Deviation from Plane

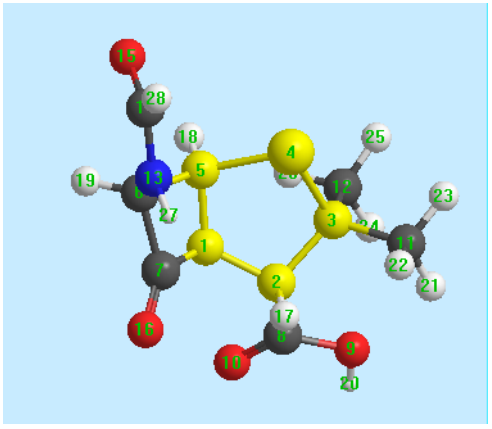
The Deviation from Plane command allows you to compute the RMS Deviation from the least squares plane fitted to the selected atoms in the model.

Example:

To examine the Deviation from Plane for five atoms in a penicillin molecule:

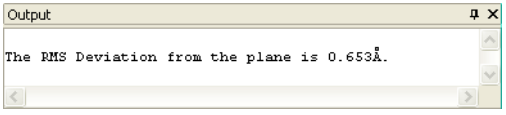
1. Build a penicillin model, as in the previous example.
2. Using the Select tool, click on the S (4) atom.
3. Shift+click the other atoms in the five-membered penicillin ring.

   The molecule should appear as follows:



4. From the Structure menu, choose Deviation from Plane.

   When the deviation from plane calculation is complete, the value appears in the Output window.



The result indicates that the atoms in the five-membered ring of penicillin are not totally coplanar; there is a slight pucker to the ring.

Removing Measurements from a Table

You can remove information from the Measurements table without affecting the model. To remove measurements from a table:

- From the Structure menu, point to Measurements and choose Clear.

Displaying the Coordinates Tables

You can view the internal coordinates or the Cartesian coordinates of your model by choosing Cartesian Table or Z-Matrix Table from the View menu.

Internal Coordinates

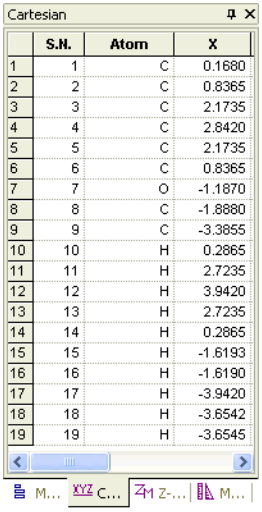
The Internal Coordinates table contains one entry for each atom. The fields contain a description of how each atom in the model is positioned relative to the other atoms in the model.

The order of atoms in the Internal Coordinates table is determined by the Z-matrix. The origin atom is listed first, and the rest of the atoms are listed in the order that they are positioned. For more information see “Scaling a Model” on page 101.

To display the Internal Coordinates table:

1. From the View menu choose Z-Matrix Table.

   The Internal Coordinates table appears.



NOTE: *The default condition is that all of the tables open in a tabbed window when you select any one.*

When you select a record in the Internal Coordinates table, the corresponding atom is selected in the model. When you select atoms in the model, the corresponding records are selected in the Internal Coordinates table.

To edit measurements in the Z-matrix:

1. Type a new measurement in the selected cell.
2. Press the Enter key.

To change which atoms Chem3D uses to position each atom use the commands in the Set Z-matrix submenu in the Structure menu.

Cartesian Coordinates

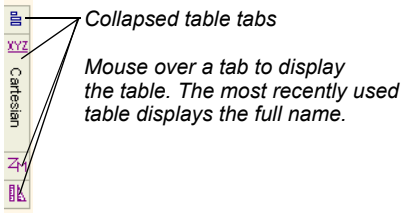
The fields in the Cartesian Coordinates table contain the atom name and the X-, Y- and Z-coordinates for each atom. The order of atoms is determined by their serial numbers. All of the atoms in a fragment are listed in consecutive records. Hydrogen, lone pair and dummy atoms are listed after heavy atoms.

To display the Cartesian Coordinates table, do one of the following:

- If the Tables window has been activated, click the XYZ tab at the bottom of the window.
- If the Tables window has not been activated, choose Cartesian Table from the View menu.

  The Cartesian Coordinates table appears.

The Cartesian Coordinates table acts like the other tables: you can select atoms or bonds either in the table or in the model. Use the pin icon to collapse the window to save space.


Collapsed table tabs
Mouse over a tab to display the table. The most recently used table displays the full name.
XYZ
Cartesian

Comparing Models by Overlay

The Overlay submenu on the Structure menu is used to lay one fragment in a model window over a second fragment. Each fragment remains rigid during the overlay computation.

Common uses of Overlay include:

- Comparing structural similarities between models with different composition.
- Comparing conformations of the same model.

Chem3D provides two overlay techniques. "Tutorial 6: Overlaying Models" on page 43 describes the Fast Overlay method. This section uses the same example—superimposing a molecule of Methamphetamine on a molecule of Epinephrine (Adrenalin) to demonstrate their structural similarities—to describe the Minimization Method.

1. From the File menu, choose New Model.
2. Select the Text Building tool and click in the model window.

   A text box appears.
3. Type Epinephrine and press the Enter key.

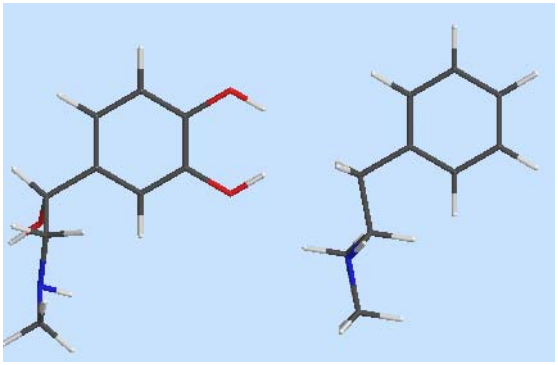
   A molecule of Epinephrine appears.
4. Click in the model window, *below* the Epinephrine molecule.

   A text box appears.
5. Type Methamphetamine and press the Enter key.

   A molecule of Methamphetamine appears beneath the Epinephrine molecule.
6. From the Model Display submenu of the View menu, deselect Show Hs and Lps.

   The hydrogen atoms and lone pairs in the molecule are hidden.

   The two molecules should appear as shown in the following illustration. You may need to move or rotate the models to display them as shown.



TIP: *To move only one of the models, select an atom in it before rotating.*

7. From the Model Display submenu of the View menu, select Show Atom Labels and Show Serial Numbers.

   The atom labels and serial numbers appear for all the visible atoms.

To perform an overlay, you must first identify atom pairs by selecting an atom in each fragment, and then display the atom pairs in the Measurements table.

Atom Pair —an atom in one fragment which has a distance specified to an atom in a second fragment.

1. Select C(9) in the Epinephrine molecule.
2. Shift+click C(27) in the Methamphetamine molecule.
3. From the Structure menu, point to Measurements and choose Set Distance.

   The Measurements table appears. The Actual cell contains the current distance between the two atoms listed in the Atom cell.
4. For an acceptable overlay, you must specify at least three atom pairs, although it can be done with only two pairs. Repeat steps 1 to 3 to create at least three atom pairs.
5. The optimal distances for overlaying two fragments are assumed to be zero for any atom pair that appears in the Measurements table. For each atom pair, type 0 into the Optimal column and press the Enter key.

Your measurements table should look something like this:

Measurement

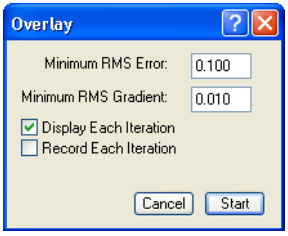
	Atoms	Actual	Optimal
1	C(9)-C(27)	8.2774	0.0000
2	N(28)-N(8)	8.1075	0.0000
3	C(31)-C(5)	8.1876	0.0000
4	C(33)-C(10)	8.1936	0.0000
5	C(2)-C(36)	8.1933	0.0000

Now perform the overlay computation:

> ***NOTE:*** *To help see the two overlaid fragments, you can color a fragment. For more information see "Working With the Model Explorer" on page 111*

1. From the Model Display submenu of the View menu, deselect Show Atom Labels and Show Serial Numbers.
2. From the Structure menu point to Overlay, and click Minimize.

   The Overlay dialog box appears.



3. Type 0.100 for the Minimum RMS Error and 0.010 for the Minimum RMS Gradient.

   The overlay computation will stop when either the RMS Error becomes less than the Minimum RMS Error or the RMS Gradient becomes less than the Minimum RMS Gradient value.
4. Click Display Every Iteration.
5. Click Start.

   How the fragments are moved at each iteration of the overlay computation is displayed.

To save the iterations as a movie, click the Record Each Iteration check box.

To stop the overlay computation before it reaches the preset minima, click Stop Calculation on the toolbar.

The Overlay operation stops. Recording is also stopped.

The following illustration shows the distances between atom pairs at the completion of the overlay computation. The distances in the Actual cells are quite close to zero.

Measurement

	Atoms	Actual	Optimal
1	C(9)-C(27)	0.4872	0.0000
2	N(28)-N(8)	0.6404	0.0000
3	C(31)-C(5)	0.0995	0.0000
4	C(33)-C(10)	0.1653	0.0000
5	C(2)-C(36)	0.1021	0.0000

Your results may not exactly match those described. The relative position of the two fragments or molecules at the start of the computation can affect the final results.

Working With the Model Explorer

The Model Explorer displays a hierarchical tree representation of the model. It provides an easy way to explore the structure of any model, even complex macromolecules, and alter display properties at any level.

The Model Explorer defines the model in terms of "objects". Every object has a set of properties, including a property that defines whether or not it belongs to another object (is a "child" of a higher level "parent" object.)

The default setting for all properties is Inherit Setting. This means that "parents" determine the properties of "children", until you choose to

change a property. By changing some property of a lower level object, you can better visualize the part of the model you want to study.

Use the Model Explorer to:

- Define objects.
- Add objects to groups.
- Rename objects.
- Delete objects, with or without their contents.

The display properties of objects you can alter include:

- Changing the display mode.
- Showing or hiding.
- Changing the color.

At the atom level, you can display or hide:

- Atom spheres
- Atom dots
- Element symbols
- Serial numbers

Model Explorer Objects

The Model Explorer objects are:

- Fragments
- Chains
- Groups
- Atoms
- Bonds
- Solvents
- Backbone

The Fragment object represents the highest level segment ("parent") of a model. Fragments represent separate parts of the model, that is, if you start at an atom in one fragment, you cannot trace through a series of bonds that connect to an atom in another fragment. If you create a bond between two such atoms, Chem3D will collapse the hierarchical structure to create one fragment.

Fragment objects typically consist of chains and groups, but may also contain individual atoms and bonds.

In Chem3D, chains and groups are functionally identical. Chains are special groups found in PDB files. If you rename a group as a chain, or vice versa, the icon will change. This is also the reason that only the work "Group" is used in the menus. All Group commands also apply to chains.

Group objects can consist of other groups, atoms and bonds. Chem3D does not limit a group to contiguous atoms and bonds, though this is the logical definition.

Bond objects do not appear by default in the Model Explorer. If you want to display bonds, select Show Bonds in the GUI tab of the Chem3D Preferences dialog box.

The Solvent object is a special group containing all of the solvent molecules in the model. The individual molecules appear as "child" groups within the Solvent object. A Solvent object should not be child of any other object.

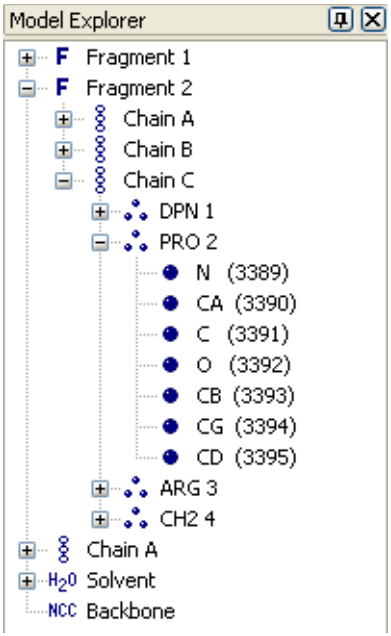
NOTE: *When importing PDB models, solvents will sometimes show up in chains. While this is incorrect, Chem3D preserves this structure in order to be able to save the PDB file again.*

The Backbone object is a display feature that allows you to show the carbon-nitrogen backbone structure of a protein. It appears in the Model Explorer as a separate object with no children. The atoms and bonds that make up the backbone belong to other chains and groups, but are also virtual children of the Backbone object. This allows you to select display properties for the backbone that override the display properties of the chains and groups above them in the hierarchy.

To display the Model Explorer:

- From the View menu choose Model Explorer.

The Model Explorer window appears along the left side of the model.

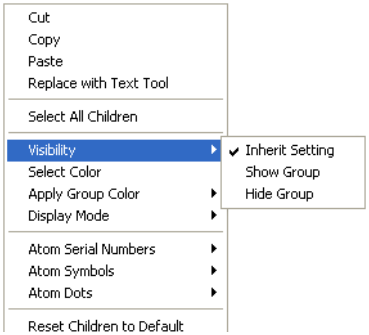


To view or change a property in a model:

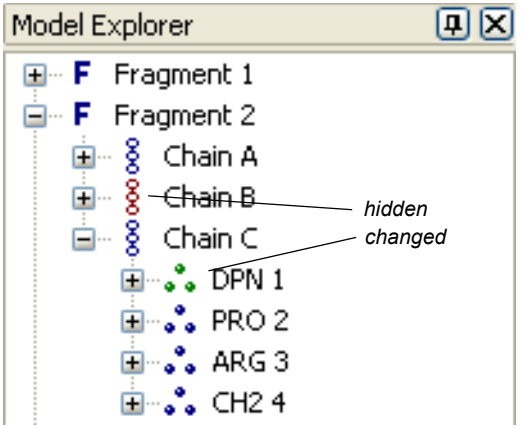
1. Select the object (fragment, group, or atom) you wish to change.

   TIP: *To select multiple objects, use Shift+click if they are contiguous or Ctrl+click if they are not.*

2. Right-click, select the appropriate submenu, and choose a command.



When you change an object property, the object icon changes to green. When you hide an object, the icon changes to red. Objects with default properties have a blue icon.



Creating Groups

Some models, PDB proteins for example, have group information incorporated in the file. For other models you will need to define the groups. To do this in the Model Explorer:

1. Holding down the Ctrl key, select the atoms in the group.
2. Choose New Group from the Context-Sensitive menu.

   The group is created with the default name selected.
3. Rename the group by typing a new name.

Adding to Groups

You can add lower level objects to an existing group, or combine groups to form new groups.

To add to a group:

1. Select the objects you want to combine, using either Shift+click (contiguous) or Ctrl+click (non-contiguous).
2. Select Move Objects to Group from the Right-click menu.
3. Rename the group, if necessary.

> ***NOTE:*** *The order of selection is important. The group or chain you are adding to should be the last object selected.*

Pasting Substructures

You can cut-and-paste or copy-paste any substructure into another structure, either within or between model windows. In addition to the usual methods—using the Cut, Copy, and Paste commands on either the Edit or Context-Sensitive menus, or Ctrl+X, Ctrl+C, and Ctrl+V—you can use the Text tool to paste substructures.

To paste a substructure with the Text tool:

1. Select a fragment, chain, or group.
2. Choose Replace with Text Tool from the Context-Sensitive menu.

   The substructure appears in a Text tool in the model window.
3. Click the Text tool on the atom that you want to link to the substructure.

Deleting Groups

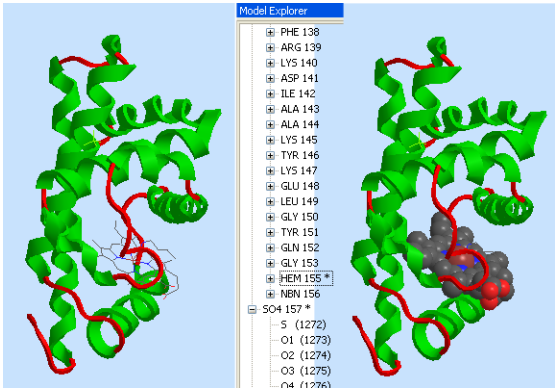
When deleting groups, you have two options:

If you want to...	Then Select...
remove the grouping, but leave the model intact	Delete Group
delete the group from the model	Delete Group and Contents

Using the Display Mode

One means of bringing out a particular part of a model is by changing the display mode. The usual limitations apply (see "Model Types" on page 56). The submenu will only display available modes.

The following illustration shows the effect of changing the HEM155 group of PDB-101M from Wireframe (the default) to Space Filling.



Coloring Groups

Another means of visualization is by assigning different colors to groups. Changing a group color in the Model Explorer overrides the standard color settings in the Elements table and the Substructures table.

To change a group color:

1. Select a group or groups.
2. Choose Select Color on the Right-click menu.

   The Color Dialog box appears.
3. Choose a color and click OK.

The Apply Group Color command is automatically selected.

To revert to the default color:

1. Select a group or groups.
2. Right-click, point to Apply Group Color on the Context-Sensitive menu and select Inherit Group Color.

   The default group color is displayed.

Resetting Defaults

To remove changes, use the Reset All Children command.

Animations

You can animate iterations from computations by saving frames in a movie.You control the creation and playback of movies from the Movie menu or toolbar.

Creating and Playing Movies

To display the Movie toolbar:

- From the View menu, point to Toolbars and choose Movies.

  The Movie toolbar appears.

To create a movie, select the Record Every Iteration checkbox when you set up the calculation.

To stop recording click Stop Calculations on the Calculation toolbar Movie, or let the calculation terminate according to preset values.

To view different frames of your movie:

1. Click the arrow on the Position button of the Movie toolbar.

   The Movie Process tool appears.

TIP: *You can tear the toolbar off by dragging the title bar.*

2. Drag the Slider knob to the frame you wish to view.

TIP: *You can also use the Previous and Next buttons to locate a frame in the movie.*

To play back a movie you created:

- Click Start.

To stop playback of a movie:

- Click Stop.

Spinning Models

You can spin models about a selected axis. The number of frames created when you choose a Spin command is set using the Smoothness Slider in the Movies control panel.

Spin About Selected Axis

To spin the model around an axis specified by a selection:

- Choose Spin About... from the Movie menu.

  The Spin About... command automatically activates the Record command.

To stop spinning:

- On the Movie toolbar, click the Stop button.

  Spins are automatically recorded.

To replay the spins:

- Click Start.

Editing a Movie

You can change a movie by removing frames.

To remove a frame:

1. Position the movie to the frame you want to delete.
2. Click the Remove Frame button.

Movie Control Panel

You can control how a movie is created by changing settings in the Movies control panel in the Model Settings dialog box. You can specify the number of frames and at what increment they are captured.

To display the Movies control panel:

1. From the Movies menu, choose Properties.
2. Take the appropriate actions:

If you want to ...	Then ...
set the movie to loop or repeat backwards and forwards	Click the Loop or Back and Forth radio button.
specify the speed at which the movie is replayed	Drag the Speed slider knob to the left to play your movie at a slower speed (a smaller number of degrees per second). Drag the Speed slider knob to the right to play your movie at a faster speed (a larger number of degrees per second).
specify the number of degrees of rotation that is captured as a frame while recording.	Drag the Smoothness slider knob to the left to capture more frames (a smaller number of degrees of rotation capture a frame). Drag the Smoothness slider knob to the right to capture fewer frames (a larger number of degrees of rotation capture a frame).

Chapter 7: Printing and Exporting Models

Printing Models

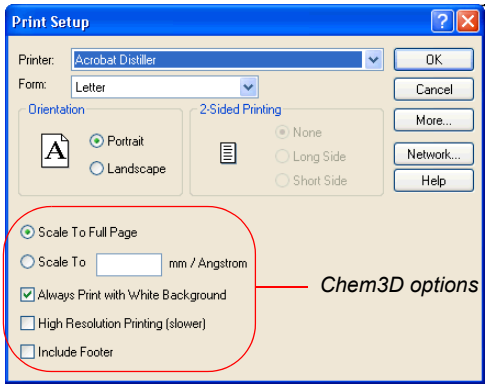
You can print Chem3D models to PostScript and non-PostScript printers. Before printing you can specify options about the print job.

Specifying Print Options

To prepare your model for printing:

1. From the File menu, choose Print Setup.

   The Print Setup dialog box appears. The available options depend on the printer you use. There are five options specific to Chem3D, which are described in the following table.



2. Select the appropriate options:

If you want to ...	Then select ...
resize your model according to a scaling factor	Scale To and type a scaling value. Scaling factors are measured in pixels per angstrom. A pixel is 1/72 of an inch, or approximately 1/28 of a centimeter. With a value of 28 pixels/Ångstrom your model is scaled so that a distance of one Ångstrom in the model is 1 centimeter in the printed image. If you specify a value of 72 pixels/angstrom, a distance of one angstrom in the model is scaled to 1 inch on the printed image.
scale your model so the printed image fills the printed page	Scale To Full Page.
print with white background (default)	Always Print with White Background

If you want to ...	Then select ...
produce publication quality output.	High Resolution Printing (this can also be set with the OpenGL Preferences settings.)
print a footer at the bottom left of the printed page containing the name of the model and the date and time changes were last made	Include Footer.

Printing

To print the contents of the active window:

- From the File menu, choose Print.

  The Print dialog box appears. The contents of the dialog box depend upon the type of printer you are using.

The picture of the model is scaled according to the settings in the Page Setup dialog box.

To print a table, right-click in the table and select Print.

Exporting Models Using Different File Formats

The following table shows all of the chemistry file formats supported by Chem3D. For more information about file formats, see "Appendix E: File Formats."

File Format	Name	Extension
Alchemy	Alchemy	.alc; .mol
Cartesian Coordinate	Cart Coords 1	.cc1
	Cart Coords 2	.cc2
CCDB	Cambridge Crystallographic Database	.ccd
Chem3D		.c3xml; .c3d
Chem3D template		.c3t
ChemDraw	ChemDraw	.cdx; .cdxml
Connection Table	Conn Table	.ct; .con
GAMESS Input	GAMESS Input	.inp
Gaussian Checkpoint		.fchk; .fch
Gaussian Cube		.cub
Gaussian Input	Gaussian Input	.gjc; .gjf
Internal Coordinates	Int Coords	.int
MacroModel	MacroModel	.mcm; .dat; .out

File Format	Name	Extension
Molecular Design Limited MolFile	MDL MolFile	.mol
MSI ChemNote	MSI ChemNote	.msm
MOPAC input file	MOPAC	.mop; .dat; .mpc; 2mt
MOPAC graph file		.gpt
Protein Data Bank	Protein DB	.pdb; .ent
ROSDAL	Rosdal	.rdl
Standard Molecular Data	SMD File	.smd
SYBYL MOL	SYBYL	.sml
SYBYL MOL2	SYBYL2	.sm2; .ml2
Tinker	MM2; MM3	.xyz

To save a model with a different format, name or location:

1. From the File menu, choose **Save As**.

   The Save File dialog box appears.
2. Specify the name of the file, the folder, and disk where you want to save the file.
3. Select the file format in which you want to save the model.
4. Click Save.

When you save a file in another file format, only information relevant to the file format is saved. For example, you will lose dot surfaces, color, and atom labels when saving a file as an MDL MolFile.

Publishing Formats

The following file formats are used to import and/or export models as pictures for desktop publishing and word processing software.

WMF and EMF

Chem3D supports the Windows Metafile and Enhanced Metafile file formats. These are the only graphic formats (as opposed to chemistry modeling formats) that can be used for import. They may also be used for export, EMF by using the Save As... File menu command or the clipboard, and WMF by using the clipboard (only). See "Exporting With the Clipboard" on page 127 for more information. EMF files are exported with transparent backgrounds, when this is supported by the operating system (Windows 2000 and Windows XP). The WMF and EMF file formats are supported by applications such as Microsoft Word for Windows.

NOTE: *Chem3D no longer embeds structural information in models exported as EMF files. If you have EMF files produced with previous versions of Chem3D, you can still open them in Chem3D and work with the structure. However, EMF files saved from Chem3D 8.0 contain graphic information only and cannot be opened in Chem3D 8.0.*

BMP

The Bitmap file format saves the bitmapped representation of a Chem3D picture. The Bitmap file format enables you to transfer Chem3D pictures to other applications, such as Microsoft Word for Windows, that support bitmaps.

EPS

The PostScript file format saves models as encapsulated postscript file (EPS). EPS files are ASCII text files containing the scaleable PostScript representation of a Chem3D picture. You can open EPS files using other applications such as PageMaker. You can transfer EPS files among platforms, including Macintosh, Windows, and UNIX.

TIF

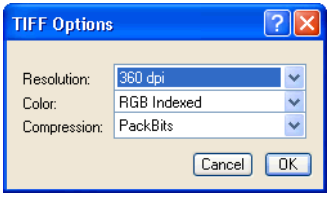
The Tagged Image File Format (TIFF) contains binary data describing a bitmap image of the model. TIFF is a high resolution format commonly used for saving graphics for cross-platform importing into desktop publishing applications. TIFF images can be saved using a variety of resolution, color, and compression options. As TIFF images can get large, choosing appropriate options is important.

When you save a file as .TIF, an option button appears in the Save As dialog box.

To specify the save options:

1. Click Options:

   The TIFF Options dialog box appears.



2. Choose a resolution. The size of the file increases as the square of the resolution.
3. Choose a color option.

If you want to ...	Then choose ...
force objects to black and white.	Monochrome.
store colors using computer monitor style of color encoding.	RGB Indexed.
use printing press style of color encoding.	CMYK Contiguous. Stores colors non-sequentially. For example: CMYKCMYK. The PackBits compression type provides no compression for this type of file.

NOTE: *If objects in your document are black and white they are saved as black and white regardless of which Color options you set. If you import drawings from other applications and want them to print Black and White you must set the Color option to Monochrome.*

4. Choose a compression option:

If you want to ...	Then choose ...
reduce file size by encoding repeating bytes of information as output. For example, for a line of color information such as: CCCCCMMMMMYYYYYKKKKK, the compression yields a smaller file by representing the information as C5M5Y5K5.	PackBits.
fax transmissions of images	CCITT Group 3 or CCITT Group 4.

GIF and PNG and JPG

Use the Graphics Interchange Format (GIF), Portable Network Graphics (PNG) file format, or the JPEG format to publish a Chem3D model on the world wide web. Each of these formats uses a compression algorithm to reduce the size of the file. Applications that can import GIF, PNG, and JPG files include Netscape Communicator and Microsoft Internet Explorer.

The model window background color is used as the transparent color in the GIF format graphic.

NOTE: *The size of the image in Chem3D when you save the file will be the size of the image as it appears in your web page. If you turn on the "Fit Model to Window" building preference in Chem3D, you can resize the Chem3D window (in Chem3D) to resize the model to the desired size and then save.*

3DM

The QuickDraw 3D MetaFile (3DM) file format contains 3-dimensional object data describing the model. You can import 3DM files into many 3D modeling applications. You can transfer 3DM files between Macintosh and Windows platforms.

AVI

Use this file format to save a movie you have created for the active model. You can import the resulting movie file into any application that supports the AVI file format.

Formats for Chemistry Modeling Applications

The following file formats are used to export models to chemistry modeling application other than Chem3D. Most of the formats also support import.

Alchemy

Use the ALC file format to interface with TRIPOS© applications such as Alchemy©. This is supported only for input.

Cartesian Coordinates

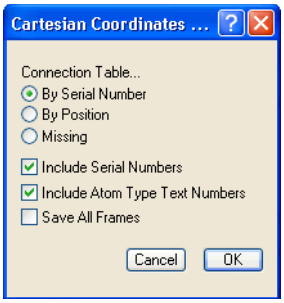
Use Cartesian Coordinates 1 (.CC1) or 2 (.CC2) to import or export the X, Y, and Z Cartesian coordinates for your model.

When you save a file as Cartesian Coordinates, an option button appears in the Save As dialog box.

To specify the save options:

1. Click Options:

   The Cartesian Coordinates Options dialog box appears.



2. Select the appropriate options:

If you want the file to ...	Then click ...
contain a connection table for each atom with serial numbers	By Serial Number.
contain a connection table for each atom that describes adjacent atoms by their positions in the file	By Position.
not contain a connection table	Missing.

If you want the file to ...	Then click ...
contain serial numbers	Include Serial Numbers.
contain atom type numbers	Include Atom Type Text Numbers.
contain internal coordinates for each view of the model	Save All Frames.

Connection Table

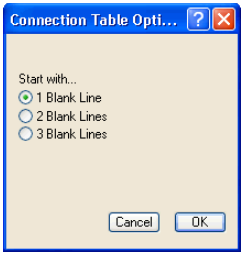
Chem3D uses the atom symbols and bond orders of connection table files to guess the atom symbols and bond orders of the atom types. There are two connection table file formats, CT and CON. The CON format is supported only for import.

When you save a file as a Connection Table, an Options button appears in the Save As dialog box.

To specify the save options:

1. Click Options.

   The Connection Table Options dialog box appears.



2. Select the appropriate options:

If you want to add ...	Then click ...
a blank line to the top of the file	1 Blank Line.
two blank lines to the top of the file	2 Blank Lines.
three blank lines to the top of the file	3 Blank Lines.

Gaussian Input

Use the Gaussian Input (GJC, GJF) file format to interface with models submitted for Gaussian calculations. Either file format may be used to import a model. Only the Molecule Specification section of the input file is saved. For atoms not otherwise specified in Chem3D, the charge by default is written as 0, and the spin multiplicity is written as 1. You can edit Gaussian Input files using a text editor with the addition of keywords and changing optimization flags for running the file using the Run Gaussian Input file within Chem3D, or using Gaussian directly.

Gaussian Checkpoint

A Gaussian Checkpoint file (FCHK; FCH) stores the results of Gaussian Calculations. It contains the final geometry, electronic structure (including energy levels) and other properties of the molecule. Checkpoint files are supported for import only.

Chem3D displays atomic orbitals and energy levels stored in Checkpoint files. If Cubegen is installed, molecular surfaces are calculated from the Checkpoint file.

Gaussian Cube

A Gaussian Cube file (CUB) results from running Cubegen on a Gaussian Checkpoint file. It contains information related to grid data and model coordinates. Gaussian Cube files are supported for import only.

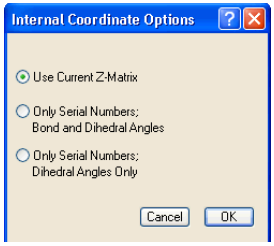
Chem3D displays the surface the file describes. If more than one surface is stored in the file, only the first is displayed. You can display additional surfaces using the Surfaces menu.

Internal Coordinates

Internal Coordinates (.INT) files are text files that describe a single molecule by the internal coordinates used to position each atom. The serial numbers are determined by the order of the atoms in the file. The first atom has a serial number of 1, the second is number 2, and so on. Internal Coordinates files may be both imported and exported.

You cannot use a Z-matrix to position an atom in terms of a later-positioned or higher serialized atom. If you choose the second or third options in the Internal Coordinates Options dialog box, the nature of the serialization of your model determines whether a consistent Z-matrix can be constructed. If the serial numbers in the Z-matrix which is about to be created are not consecutive, a message appears. You are warned if the atoms in the model must be reserialized to create a consistent Z-matrix.

When you click Options in the Save As dialog box, the following dialog box appears:



Select the appropriate options:

If you want to ...	Then click ...
save your model using the Z-matrix described in the Internal Coordinates table of the model	Use Current Z-matrix.
build a Z-matrix in which the current serial number ordering of the atoms in the model is preserved in the Z-matrix	Only Serial Numbers; Bond and Dihedral Angles. Pro-R/Pro-S and Dihedral angles are used to position atoms.
build a Z-matrix in which the current serial number ordering of the atoms in the model is preserved in the Z-matrix	Only Serial Numbers; Dihedral Angles Only. The Pro-R and Pro-S stereochemical designations are not used in constructing the Z-matrix from a model. All atoms are positioned by dihedral angles only.

MacroModel Files

The MacroModel[1] (MCM; DAT; OUT) file formats are defined in the MacroModel Structure Files version 2.0 documentation. Chem3D supports import of all three file types, and can export MCM

1. MacroModel is produced within the Department of Chemistry at Columbia University, New York, N.Y.

Molecular Design Limited MolFile (.MOL)

The MDL Molfile format saves files by MDL applications such as ISIS/Draw, ISIS/Base, MAACS and REACCS. The file format is defined in the article, "Description of Several Chemical Structure File Formats Used by Computer Programs Developed at Molecular Design Limited" in the Journal of Chemical Information and Computer Science, Volume 32, Number 3, 1992, pages
244–255.

Use this format to interface with MDL's ISIS applications and other chemistry-related applications. Both import and export are supported.

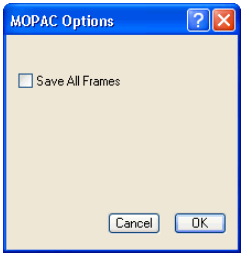
MSI ChemNote

Use the MSI ChemNote (.MSM) file format to interface with Molecular Simulations applications such as ChemNote. The file format is defined in the ChemNote documentation. Both import and export are supported.

MOPAC Files

MOPAC data may be stored in MOP, DAT, MPC, or 2MT file formats. Chem3D can import any of these file formats, and can export MOP files. You can edit MOPAC files using a text editor, adding keywords and changing optimization flags, and run the file using the Run MOPAC Input file command within Chem3D.

When you click Options in the Save As dialog box, the MOPAC options dialog box appears:



Click the Save All Frames check box to create a MOPAC Data file in which the internal coordinates for each view of the model are included. The initial frame of the model contains the first 3 lines of the usual MOPAC output file (see the example file below). Each subsequent frame contains only lines describing the Z-matrix for the atoms in that frame.

NOTE: *For data file specifications, see page 13 of the online MOPAC manual.*

To edit a file to run using the Run MOPAC Input File command:

1. Open the MOPAC output file in a text editor.

The output file below shows only the first four atom record lines. The first line and column of the example output file shown below are for purposes of description only and are not part of the output file.

	Col. 1	Col. 2	C3	Col. 4	C5	Col. 6	Col. 7	Col. 8		
Line 1										
Line 2:	Cyclohexanol									
Line 3:										
Line 4:	C	0	0	0	0	0	0	0	0	0
Line 5:	C	1.54152	1	0	0	0	0	1	0	0
Line 6:	C	1.53523	1	111.7747	1	0	0	2	1	0
L7..Ln	C	1.53973	1	109.7114	1	-55.6959	1	1	2	3
Ln+1										

2. In Line 1, type the keywords for the computations you want MOPAC to perform (blank in the example above).

   Line 2 is where enter the name that you want to assign to the window for the resulting model. However, Chem3D ignores this line.

3. Leave Line 3 blank.

4. Line 4 through Ln (were n is the last atom record) include the internal coordinates, optimization flags, and connectivity information for the model.

   - Column 1 is the atom specification.
   - Column 2 is the bond distance (for the connectivity specified in Column 8).
   - Column 3 is the optimization flag for the bond distance specified in Column 2.
   - Column 4 is the bond angle (for the connectivity specified in Column 8).
   - Column 5 is the optimization flag for the bond angle specified in Column 4.
   - Column 6 is the dihedral angle (for the connectivity specified in Column 8).
   - Column 7 is the optimization flag for the dihedral angle specified in Column 6.

5. To specify particular coordinates to optimize, change the optimization flags in Column 3, Column 5 and Column 7 for the respective internal coordinate. The available flags in MOPAC are:

1	Optimize this internal coordinate
0	Do not optimize this internal
-1	Reaction coordinate or grid index
T	Monitor turning points in DRC

6. Add additional information in line Ln+1. For example, symmetry information used in a SADDLE computation.

7. Leave the last line in the data file blank to indicate file termination.
8. Save the file in a text only format.

MOPAC Graph Files

A MOPAC Graph (GPT) file stores the results of MOPAC calculations that include the GRAPH keyword. It contains the final geometry, electronic structure, and other properties of the molecule. Chem3D supports the MOPAC Graph file format for import only.

Protein Data Bank Files

Brookhaven Protein Data Bank files (PDB; ENT) are used to store protein data and are typically large in size. Chem3D can import both file types, and exports PDB. The PDB file format is taken from the Protein Data Bank Atomic Coordinate and Bibliographic Entry Format Description.

ROSDAL Files (RDL)

The ROSDAL Structure Language[1] (RDL) file format is defined in Appendix C: ROSDAL Syntax of the MOLKICK User's Manual, and in this manual in Appendix E, "File Formats." on page 262. The ROSDAL format is primarily used for query searching in the Beilstein Online Database. Chem3D supports the ROSDAL file format for export only.

Standard Molecular Data (SMD)

Use the Standard Molecular Data (.SMD) file format for interfacing with the STN Express application for online chemical database searching. Both import and export are supported.

1. ROSDAL is a product of Softron, Inc.

SYBYL Files

Use the SYBYL© (SML, SM2, ML2) file formats to interface with Tripos's SYBYL applications. The SML and SM2 formats can be used for both import and export; the ML2 format is supported for import only.

Tinker MM2 and MM3 Files

Use the XYZ file format to interface with TINKER© software tools. Specify MM2 for most models, MM3 for proteins. Both import and export are supported.

Job Description File Formats

You can use Job description files to save customized default settings for calculations. You can save customized calculations as a Job Description file (.JDF) or Job Description Stationery (.JDT). Saving either format in a Chem3D job folder adds it to the appropriate Chem3D menu.

JDF Files

The JDF file format is a file format for saving job descriptions. When you open a JDF file, you can edit CSBR and save the settings.

JDT Files

The JDT file format is a template format for saving settings that can be applied to future calculations. You can edit the settings of a template file, however you cannot save your changes.

Exporting With the Clipboard

The size of the file that you copy to the clipboard from Chem3D is determined by the size of the Chem3D model window. If you want the size of a copied molecule to be smaller or larger, resize the model window accordingly before you copy it. If the model windows for several models are the same size, and Fit Model to Window is on, then the models should copy as the same size.

Transferring to ChemDraw

You can transfer information to ChemDraw as a 3D model or as a 2D model.

To transfer a model as a 3D picture:

1. Select the model.
2. From the Edit menu, point to Copy As, then choose Picture.
3. In ChemDraw, select Paste from the Edit menu.

> ***NOTE:*** *The model is imported as an EMF graphic and contains no structural information.*

To transfer a model as a 2D structure:

1. Select the model.
2. From the Edit menu, point to Copy As, then choose ChemDraw Structure.
3. Open ChemDraw.
4. From the Edit menu, choose Paste.

   The model is pasted into ChemDraw.

Transferring to Other Applications

To copy and paste a space-filling model into a word processing, desktop publishing, presentation or drawing application, such as Microsoft Word or PowerPoint:

1. Select the model.
2. From the Edit menu, point to Copy As, then choose **Picture**.
3. Paste the model into the target application document.

> ***TIP:*** *If you are pasting into MS Word or PowerPoint, select* Paste Special *and choose the type of graphic you wish to import: bitmap, WMF, or EMF. The EMF option will copy with a transparent background.*

Alternatively, you could use Save As Bitmap or EMF to create a file to insert into or link to the target application document.

Chapter 8: Computation Concepts

Computational Chemistry Overview

Computational chemistry extends beyond the traditional boundaries separating chemistry from physics, biology, and computer science. It allows the exploration of molecules by using a computer when an actual laboratory investigation may be inappropriate, impractical, or impossible. As an adjunct to experimental chemistry, its significance continues to be enhanced by increases in computer speed and power.

Aspects of computational chemistry include:

- Molecular modeling.
- Computational methods.
- Computer-Aided Molecular Design (CAMD).
- Chemical databases.
- Organic synthesis design.

While a number of different definitions have been proposed, the definition offered by Lipkowitz and Boyd of computational chemistry as "those aspects of chemical research that are expedited or rendered practical by computers" is perhaps the most inclusive.

Molecular modeling, while often taken to include computational methods, can be thought of as the rendering of a 2D or 3D model of a molecule's structure and properties. Computational methods, on the other hand, calculate the structure and property data necessary to render the model. Within a modeling program, such as Chem3D, computational methods are referred to as computation engines, while geometry engines and graphics engines render the model.

Chem3D supports a number of powerful computational chemistry methods and extensive visualization options.

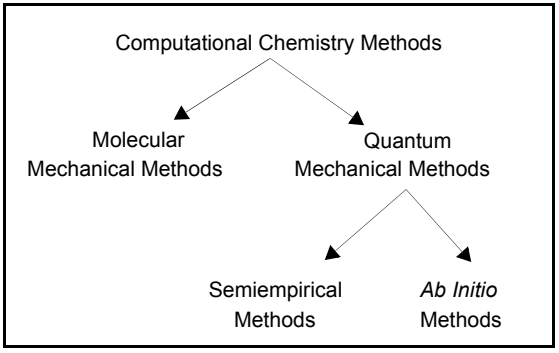
Computational Methods Overview

Computational chemistry encompasses a variety of mathematical methods which fall into two broad categories:

- **Molecular mechanics**—applies the laws of classical physics to the atoms in a molecule without explicit consideration of electrons.
- **Quantum mechanics**—relies on the Schrödinger equation to describe a molecule with explicit treatment of electronic structure.

  Quantum mechanical methods can be subdivided into two classes: *ab initio* and semiempirical.

The generally accepted method classes are shown in the following chart.



Chem3D provides the following methods:

- Molecular mechanical MM2 and MM3 method.

- Semiempirical Extended Hückel, MINDO/3, MNDO, MNDO-d, AM1 and PM3 methods through Chem3D and CS MOPAC.
- *Ab initio* methods through the Chem3D Gaussian or GAMESS interface.

Uses of Computational Methods

Computational methods calculate the potential energy surfaces (PES) of molecules. The potential energy surface is the embodiment of the forces of interaction among atoms in a molecule. From the PES, structural and chemical information about a molecule can be derived. The methods differ in the way the surface is calculated and in the molecular properties derived from the energy surface.

The methods perform the following basic types of calculations:

- **Single point energy calculation**—The energy of a given spacial arrangement of the atoms in a model or the value of the PES for a given set of atomic coordinates.
- **Geometry optimization**—A systematic modification of the atomic coordinates of a model resulting in a geometry where the net forces on the structure sum to zero. A 3-dimensional arrangement of atoms in the model representing a local energy minimum (a stable molecular geometry to be found without crossing a conformational energy barrier).
- **Property calculation**—Predicts certain physical and chemical properties, such as charge, dipole moment, and heat of formation.

Computational methods can perform more specialized functions, such as conformational searches and molecular dynamics simulations.

Choosing the Best Method

Not all types of calculations are possible for all methods and no one method is best for all purposes. For any given application, each method poses advantages and disadvantages. The choice of method depend on a number of factors, including:

- The nature of the molecule
- The type of information sought
- The availability of applicable experimentally determined parameters (as required by some methods)
- Computer resources

The three most important of the these criteria are:

- **Model size**—The size of a model can be a limiting factor for a particular method. The limiting number of atoms in a molecule increases by approximately one order of magnitude between method classes from *ab initio* to molecular mechanics. A*b initio* is limited to tens of atoms, semiempirical to hundreds, and molecular mechanics to thousands.
- **Parameter Availability**—Some methods depend on experimentally determined parameters to perform computations. If the model contains atoms for which the parameters of a particular method have not been derived, that method may produce invalid predictions. Molecular mechanics, for example, relies on parameters to define a force-field. Any particular force-field is only applicable to the limited class of molecules for which it is parametrized.
- **Computer resources**—Requirements increase relative to the size of the model for each of the methods.

  Ab initio: The time required for performing computations increases on the order of N^4, where N is the number of atoms in the model.

Semiempirical: The time required for computation increases as N^3 or N^2, where N is the number of atoms in the model.

MM2: The time required for performing computations increases as N^2, where N is the number of atoms.

In general, molecular mechanical methods are computationally less expensive than quantum mechanical methods. The suitability of each general method for particular applications can be summarized as follows.

Molecular Mechanics Methods Applications Summary

Molecular mechanics in Chem3D apply to:

- Systems containing thousands of atoms.
- Organic, oligonucleotides, peptides, and saccharides.
- Gas phase only (for MM2).

Useful techniques available using MM2 methods include:

- Energy Minimization for locating stable conformations.
- Single point energy calculations for comparing conformations of the same molecule.
- Searching conformational space by varying a single dihedral angle.
- Studying molecular motion using Molecular Dynamics.

Quantum Mechanical Methods Applications Summary

Useful information determined by quantum mechanical methods includes:

- Molecular orbital energies and coefficients.
- Heat of Formation for evaluating conformational energies.
- Partial atomic charges calculated from the molecular orbital coefficients.
- Electrostatic potential.
- Dipole moment.
- Transition-state geometries and energies.
- Bond dissociation energies.

The semiempirical methods available in Chem3D and CS MOPAC apply to:

- Systems containing up to 120 heavy atoms and 300 total atoms.
- Organic, organometallics, and small oligomers (peptide, nucleotide, saccharide).
- Gas phase or implicit solvent environment.
- Ground, transition, and excited states.

Ab initio methods, available through the Gaussian interface, apply to:

- Systems containing up to 150 atoms.
- Organic, organometallics, and molecular fragments (catalytic components of an enzyme).
- Gas or implicit solvent environment.
- Study ground, transition, and excited states (certain methods).

The following table summarizes the method types:

Method Type	Advantages	Disadvantages	Best For
Molecular Mechanics (MM2) Uses classical physics Relies on force-field with embedded empirical parameters	Least intensive computationally—fast and useful with limited computer resources Can be used for molecules as large as enzymes	Particular force field applicable only for a limited class of molecules Does not calculate electronic properties Requires experimental data (or data from *ab initio*) for parameters	Large systems (thousands of atoms) Systems or processes with no breaking or forming of bonds
Semiempirical (MOPAC) Uses quantum physics Uses experimentally derived empirical parameters Uses approximation extensively	Less demanding computationally than *ab initio* methods Capable of calculating transition states and excited states	Requires experimental data (or data from *ab initio*) for parameters Less rigorous than ab initio methods	Medium-sized systems (hundreds of atoms) Systems involving electronic transitions
ab initio (Gaussian) Uses quantum physics Mathematically rigorous—no empirical parameters	Useful for a broad range of systems Does not depend on experimental data Capable of calculating transition states and excited states	Computationally intensive	Small systems (tens of atoms) Systems involving electronic transitions Molecules or systems without available experimental data ("new" chemistry) Systems requiring rigorous accuracy

Potential Energy Surfaces

A potential energy surface (PES) can describe:

- A molecule or ensemble of molecules having constant atom composition (ethane, for example) or a system where a chemical reaction occurs.

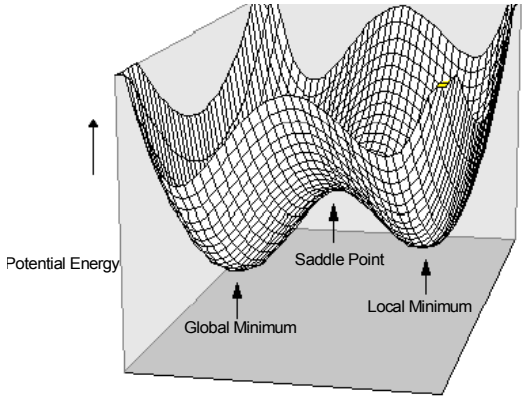
- Relative energies for conformations (eclipsed and staggered forms of ethane).

Different potential energy surfaces are generated for:

- Molecules having different atomic composition (ethane and chloroethane).
- Molecules in excited states instead of for the same molecules in their ground states.
- Molecules with identical atomic composition but with different bonding patterns, such as propylene and cyclopropane.

Potential Energy Surfaces (PES)

The true representation of a model's potential energy surface is a multi-dimensional surface whose dimensionality increases with the number of independent variables. Since each atom has three independent variables (x, y, z coordinates), visualizing a surface for a many-atom model is impossible. However, you can generalize this problem by examining any 2 independent variables, such as the x and y coordinates of an atom, as shown below.



The main areas of interest on a potential energy surface are the extrema as indicated by the arrows, are as follows:

- **Global minimum**—The most stable conformation appears at the extremum where the energy is lowest. A molecule has only one global minimum.
- **Local minima**—Additional low energy extrema. Minima are regions of the PES where a change in geometry in any direction yields a higher energy geometry.
- **Saddle point**—The point between two low energy extrema. The saddle point is defined as a point on the potential energy surface at which there is an increase in energy in all directions except one, and for which the slope (first derivative) of the surface is zero.

NOTE: *At the energy minimum, the energy is not zero; the first derivative (gradient) of the energy with respect to geometry is zero.*

All the minima on a potential energy surface of a molecule represent stable stationery points where the forces on atoms sum to zero. The global minimum represents the most stable conformation; the local minima, less stable conformations; and the saddle points represent transition conformations between minima.

Single Point Energy Calculations

Single point energy calculations can be used to calculate properties of the current geometry of a model. The values of these properties depend on where the model currently lies on the potential surface as follows:

- A single point energy calculation at a global minimum provides information about the model in its most stable conformation.
- A single point calculation at a local minimum provides information about the model in one of many stable conformations.

- A single point calculation at a saddle point provides information about the transition state of the model.
- A single point energy calculation at any other point on the potential energy surface provides information about that particular geometry, not a stable conformation or transition state.

Single point energy calculations can be performed before or after performing an optimization.

NOTE: *Do not compare values from different methods. Different methods rely on different assumptions about a given molecule.*

Geometry Optimization

Geometry optimization is used to locate a stable conformation of a model. This should be performed before performing additional computations or analyses of a model.

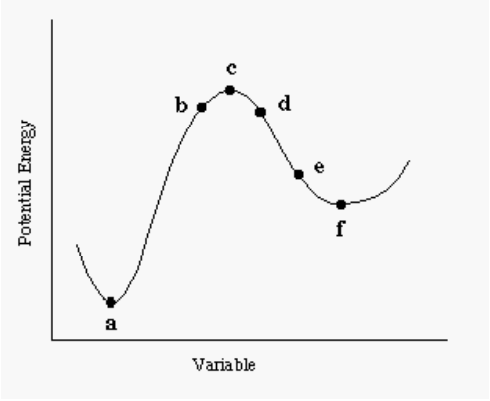
Locating global and local energy minima is often accomplished through energy minimization. Locating a saddle point is optimizing to a transition state.

The ability of a geometry optimization to converge to a minimum depends on the starting geometry, the potential energy function used, and the settings for a minimum acceptable gradient between steps (convergence criteria).

Geometry optimizations are iterative and begin at some starting geometry as follows:

1. The single point energy calculation is performed on the starting geometry.
2. The coordinates for some subset of atoms are changed and another single point energy calculation is performed to determine the energy of that new conformation.
3. The first or second derivative of the energy (depending on the method) with respect to the atomic coordinates determines how large and in what direction the next increment of geometry change should be.
4. The change is made.
5. Following the incremental change, the energy and energy derivatives are again determined and the process continues until convergence is achieved, at which point the minimization process terminates.

The following illustration shows some concepts of minimization. For simplicity, this plot shows a single independent variable plotted in two dimensions.



The starting geometry of the model determines which minimum is reached. For example, starting at (b), minimization results in geometry (a), which is the global minimum. Starting at (d) leads to geometry (f), which is a local minimum.The proximity to a minimum, but not a particular minimum, can be controlled by specifying a minimum gradient that should be reached. Geometry (f), rather than geometry (e), can be reached by decreasing the value of the gradient where the calculation ends.

Often, if a convergence criterion (energy gradient) is too lax, a first-derivative minimization can result in a geometry that is near a saddle point. This

occurs because the value of the energy gradient near a saddle point, as near a minimum, is very small. For example, at point (c), the derivative of the energy is 0, and as far as the minimizer is concerned, point (c) is a minimum. First derivative minimizers cannot, as a rule, surmount saddle points to reach another minimum.

NOTE: *If the saddle point is the extremum of interest, it is best to use a procedure that specifically locates a transition state, such as the CS MOPAC Pro Optimize To Transition State command.*

You can take the following steps to ensure that a minimization has not resulted in a saddle point.

- The geometry can be altered slightly and another minimization performed. The new starting geometry might result in either (a), or (f) in a case where the original one led to (c).
- The Dihedral Driver can be employed to search the conformational space of the model. For more information, see "Tutorial 5: Mapping Conformations with the Dihedral Driver" on page 42.
- A molecular dynamics simulation can be run, which will allow small potential energy barriers to be crossed. After completing the molecular dynamics simulation, individual geometries can then be minimized and analyzed. For more information see Appendix 9: "MM2 and MM3 Computations"

You can calculate the following properties with the computational methods available through Chem3D using the PES:

- Steric energy
- Heat of formation
- Dipole moment
- Charge density
- COSMO solvation in water
- Electrostatic potential
- Electron spin density
- Hyperfine coupling constants
- Atomic charges
- Polarizability
- Others, such as IR vibrational frequencies

Molecular Mechanics Theory in Brief

Molecular mechanics describes the energy of a molecule in terms of a set of classically derived potential energy functions. The potential energy functions and the parameters used for their evaluation are known as a "force-field".

Molecular mechanical methods are based on the following principles:

- Nuclei and electrons are lumped together and treated as unified atom-like particles.
- Atom-like particles are typically treated as spheres.
- Bonds between particles are viewed as harmonic oscillators.
- Non-bonded interactions between these particles are treated using potential functions derived using classical mechanics.
- Individual potential functions are used to describe the different interactions: bond stretching, angle bending, and torsional (bond twisting) energies, and through-space (non-bonded) interactions.
- Potential energy functions rely on empirically derived parameters (force constants, equilibrium values) that describe the interactions between sets of atoms.
- The sum of interactions determine the spatial distribution (conformation) of atom-like particles.

- Molecular mechanical energies have no meaning as absolute quantities. They can only be used to compare relative steric energy (strain) between two or more conformations of the same molecule.

The Force-Field

Molecular mechanics typically treats atoms as spheres, and bonds as springs. The mathematics of spring deformation (Hooke's Law) is used to describe the ability of bonds to stretch, bend, and twist. Non-bonded atoms (greater than two bonds apart) interact through van der Waals attraction, steric repulsion, and electrostatic attraction and repulsion. These properties are easiest to describe mathematically when atoms are considered as spheres of characteristic radii.

The total potential energy, E, of a molecule can be described by the following summation of interactions:

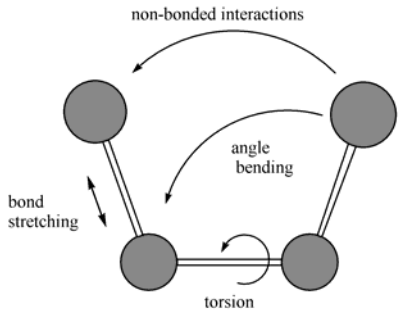
Energy = Stretching Energy + Bending Energy + Torsion Energy + Non-Bonded Interaction Energy

The first three terms, given as 1, 2, and 3 below, are the so-called bonded interactions. In general, these bonding interactions can be viewed as a strain energy imposed by a model moving from some ideal zero strain conformation. The last term, which represents the non-bonded interactions, includes the two interactions shown below as 4 and 5.

The total potential energy can be described by the following relationships between atoms. The numbers indicate the relative positions of the atoms.

1. Bond Stretching: (1-2) bond stretching between directly bonded atoms
2. Angle Bending: (1-3) angle bending between atoms that are geminal to each other.
3. Torsion Energy: (1-4) torsional angle rotation between atoms that are vicinal to each other.
4. Repulsion for atoms that are too close and attraction at long range from dispersion forces (van der Waals interaction).
5. Interactions from charges, dipoles, quadrupoles (electrostatic interactions).

The following illustration shows the major interactions.



Different kinds of force-fields have been developed. Some include additional energy terms that describe other kinds of deformations, such as the coupling between bending and stretching in adjacent bonds, in order to improve the accuracy of the mechanical model.

The reliability of a molecular mechanical force-field depends on the parameters and the potential energy functions used to describe the total energy of a model. Parameters must be optimized for a particular set of potential energy functions, and thus are not easily transferable to other force fields.

MM2

Chem3D uses a modified version of Allinger's MM2 force field. For additional MM2 references see Appendix 9: "MM2 and MM3 Computations"

The principal additions to Allinger's MM2 force field are:

- A charge-dipole interaction term
- A quartic stretching term

- Cutoffs for electrostatic and van der Waals terms with 5th order polynomial switching function
- Automatic pi system calculations when necessary
- Torsional and non-bonded constraints

Chem3D stores the parameters used for each of the terms in the potential energy function in tables. These tables are controlled by the Table Editor application, which allows viewing and editing of the parameters.

Each parameter is classified by a Quality number. This number indicates the reliability of the data. The quality ranges from 4, where the data are derived completely from experimental data (or *ab initio* data), to 1, where the data are guessed by Chem3D.

The parameter table, MM2 Constants, contains adjustable parameters that correct for failings of the potential functions in outlying situations.

NOTE: *Editing of MM2 parameters in the Table Editor should only be done with the greatest of caution by expert users. Within a force-field equation, parameters operate interdependently; changing one normally requires that others be changed to compensate for its effects.*

Bond Stretching Energy

The bond stretching energy equation is based on Hooke's law. The K_s parameter controls the stiffness of the spring's stretching (bond stretching force constant), while r_o defines its equilibrium length (the standard measurement used in building models). Unique K_s and r_o parameters are assigned to each pair of bonded atoms based on their atom types (C-C, C-H, O-C). The parameters are stored in the Bond Stretching parameter table. The constant, 71.94, is a conversion factor to obtain the final units as kcal/mole.

The result of this equation is the energy contribution associated with the deformation of a bond from its equilibrium bond length.

This simple parabolic model fails when bonds are stretched toward the point of dissociation. The Morse function would be the best correction for this problem. However, the Morse Function leads to a large increase in computation time. As an alternative, cubic stretch and quartic stretch constants are added to provide a result approaching a Morse-function correction.

The cubic stretch term allows for an asymmetric shape of the potential well, allowing these long bonds to be handled. However, the cubic stretch term is not sufficient to handle abnormally long bonds. A quartic stretch term is used to correct problems caused by these very long bonds. With the addition of the cubic and quartic stretch term, the equation for bond stretching becomes:

Both the cubic and quartic stretch constants are defined in the MM2 Constants table.

To precisely reproduce the energies obtained with Allinger's force field: set the cubic and quartic stretching constant to "0" in the MM2 Constants tables.

Angle Bending Energy

The bending energy equation is also based on Hooke's law. The K_b parameter controls the stiffness of the spring's bending (angular force

constant), while θ_0 defines the equilibrium angle. This equation estimates the energy associated with deformation about the equilibrium bond angle. The constant, 0.02191418, is a conversion factor to obtain the final units as kcal/mole.

Unique parameters for angle bending are assigned to each bonded triplet of atoms based on their atom types (C-C-C, C-O-C, C-C-H). For each triplet of atoms, the equilibrium angle differs depending on what other atoms the central atom is bonded to. For each angle there are three possibilities: XR2, XRH or XH2. For example, the XH2 parameter would be used for a C-C-C angle in propane, because the other atoms the central atom is bonded to are both hydrogens. For isobutane, the XRH parameter would be used, and for 2,2-dimethylpropane, the XR2 parameter would be used.

The effect of the K_b and θ_0 parameters is to broaden or steepen the slope of the parabola. The larger the value of K_b, the more energy is required to deform an angle from its equilibrium value. Shallow potentials are achieved with K_b values less than 1.0.

A sextic term is added to increase the energy of angles with large deformations from their ideal value. The sextic bending constant, SF, is defined in the MM2 Constants table. With the addition of the sextic term, the equation for angle bending becomes:

> ***NOTE:*** *The default value of the sextic force constant is 0.00000007. To precisely reproduce the energies obtained with Allinger's force field: set the sextic bending constant to "0" in the MM2 Constants tables.*

There are three parameter tables for the angle bending parameters:

- Angle Bending parameters
- 3-Membered Ring Angle Bending parameters
- 4-Membered Ring Angle Bending parameters

There are three additional angle bending force constants available in the MM2 Constants window. These force constants are specifically for carbons with one or two attached hydrogens. The following force constants are available.

The numbers refer to atom types, which can be found in the Atom Types Table in Chem3D.

- -CHR- Bending K for 1-1-1 angles
- -CHR- Bending K for 1-1-1 angles in 4-membered rings.
- -CHR- Bending K for 22-22-22 angles in 3-membered rings.

The -CHR- Bending K_b for 1-1-1 angles allows more accurate force constants to be specified for Type 1 (-CHR-) and Type 2 (-CHR-) interactions. The -CHR-Bending K_b for 1-1-1 angles in 4-membered rings and the -CHR- Bending K_b for 22-22-22 angles (22 is the atom type number for C Cyclopropane) in 3-membered rings differ from the -CHR- Bending K_b for 1-1-1 angles and require separate constants for accurate specification.

Torsion Energy

This term accounts for the tendency for dihedral angles (torsionals) to have an energy minimum occurring at specific intervals of 360/n. In Chem3D, n can equal 1, 2, or 3.

The $V_n/2$ parameter is the torsional force constant. It determines the amplitude of the curve. The n signifies its periodicity. $n\phi$ shifts the entire curve

about the rotation angle axis. The parameters are determined through curve-fitting techniques. Unique parameters for torsional rotation are assigned to each bonded quartet of atoms based on their atom types (C-C-C-C, C-O-C-N, H-C-C-H).

Chem3D provides three torsional parameters tables:

- Torsional parameters
- 4-Membered ring torsions
- 3-Membered ring torsions.

Non-Bonded Energy

The non-bonded energy represents the pairwise sum of the energies of all possible interacting non-bonded atoms, i and j, within a predetermined "cut-off" distance.

The non-bonded energy accounts for repulsive forces experienced between atoms at close distances, and for the attractive forces felt at longer distances. It also accounts for their rapid falloff as the interacting atoms move farther apart by a few Ångstroms.

van der Waals Energy

Repulsive forces dominate when the distance between interacting atoms becomes less than the sum of their contact radii. In Chem3D repulsion is modeled by an equation which combines an exponential repulsion with an attractive dispersion interaction ($1/R^6$):

$$E_{\text{van der Waals}} = \sum_i \sum_j \varepsilon (290000 e^{12.5/R} - 2.2 R^6)$$

where

$$R = \frac{r_{ij}}{R_i^* + R_j^*}$$

The parameters include:

- **R_i^* and R_j^***—the van der Waals radii for the atoms
- **Epsilon (ε)**—determines the depth of the attractive potential energy well and how easy it is to push atoms together
- **r_{ij}**—which is the actual distance between the atoms

At short distances the above equation favors repulsive over dispersive interactions. To compensate for this at short distances (R=3.311) this term is replaced with:

$$E_{\text{van der Waals}} = 3.1 \sum_i \sum_j$$

The R* and Epsilon parameters are stored in the MM2 Atom Types table.

For certain interactions, values in the VDW interactions parameter table are used instead of those in the MM2 atom types table. These situations include interactions where one of the atoms is very electronegative relative to the other, such as in the case of a water molecule.

Cutoff Parameters for van der Waals Interactions

The use of cutoff distances for van der Waals terms greatly improves the computational speed for large molecules by eliminating long range, and relatively insignificant, interactions from the computation.

Chem3D uses a fifth-order polynomial switching function so that the resulting force field maintains second-order continuity. The cutoff is implemented gradually, beginning at 90% of the specified cutoff distance. This distance is set in the MM2 Constants table.

The van der Waals interactions fall off as $1/r^6$, and can be cut off at much shorter distances, for example 10Å. This cut off speeds the computations significantly, even for relatively small molecules.

NOTE: *To precisely reproduce the energies obtained with Allinger's force field: set the van der Waals cutoff constants to large values in the MM2 Constants table.*

Electrostatic Energy

The electrostatic energy is a function of the charge on the non-bonded atoms, q, their interatomic distance, r_{ij}, and a molecular dielectric expression, D, that accounts for the attenuation of electrostatic interaction by the environment (solvent or the molecule itself).

In Chem3D, the electrostatic energy is modeled using atomic charges for charged molecules and bond dipoles for neutral molecules.

There are three possible interactions accounted for by Chem3D:

- charge/charge
- dipole/dipole
- dipole/charge.

Each type of interaction uses a different form of the electrostatic equation as shown below:

charge/charge contribution

where the value 332.05382 converts the result to units of kcal/mole.

dipole/dipole contribution

where the value 14.388 converts the result from ergs/mole to kcal/mole, χ is the angle between the two dipoles μ_i and μ_j, α_i and α_j are the angles the dipoles form with the vector, r_{ij}, connecting the two at their midpoints, and D_μ is the (effective) dielectric constant.

dipole/charge contribution

where the value 69.120 converts the result to units of kcal/mole.

Bond dipole parameters, μ, for each atom pair are stored in the bond stretching parameter table. The charge, q, is stored in the atom types table. The molecular dielectric is set to a constant value between 1.0 and 5.0 in the MM2 Atom types table.

NOTE: *Chem3D does not use a distance-dependent dielectric.*

Cutoff Parameters for Electrostatic Interactions

The use of cutoff distances for electrostatic terms, as for van der Waals terms, greatly improves the computational speed for large molecules by eliminating long-range interactions from the computation.

As in the van der Waals calculations, Chem3D invokes a fifth-order polynomial switching function in order to maintain second-order continuity in the force-field. The switching function is invoked as minimum values for charge/charge, charge/dipole,

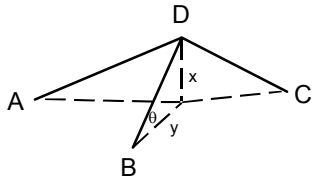
or dipole/dipole interactions are reached. These cutoff values are located in the MM2 Constants parameter table.

Since the charge-charge interaction energy between two point charges separated by a distance r is proportional to 1/r, the charge-charge cutoff must be rather large, typically 30 to 40Å, depending on the size of the molecule. The charge-dipole, dipole-dipole interactions fall off as $1/r^2$, $1/r^3$ and can be cutoff at much shorter distances, for example 25 and 18Å respectively. To precisely reproduce the energies obtained with Allinger's force field: set the cutoff constants to large values (99) in the MM2 Constants table.

OOP Bending

Atoms that are arranged in a trigonal planar fashion, as in sp^2 hybridization, require an additional term to account for out-of-plane (OOP) bending. MM2 uses the following equation to describe OOP bending:

The form of the equation is the same as for angle bending, however, the θ value used is angle of deviation from coplanarity for an atom pair and θ_o is set to zero. The illustration below shows the θ determined for atom pairs DB.



The special force constants for each atom pair are located in the Out of Plane bending parameters table. The sextic correction is used as previously described for Angle Bending. The sextic constant, SF, is located in the MM2 Constants table.

Pi Bonds and Atoms with Pi Bonds

For models containing pi systems, MM2 performs a Pariser-Parr-Pople pi orbital SCF computation for each system. A pi system is defined as a sequence of three or more atoms of types which appear in the Conjugate Pi system Atoms table. Because of this computation, MM2 may calculate bond orders other than 1, 1.5, 2, and so on.

NOTE: *The method used is that of D.H. Lo and M.A. Whitehead, Can. J. Chem., 46, 2027(1968), with heterocycle parameter according to G.D. Zeiss and M.A. Whitehead, J. Chem. Soc. (A), 1727 (1971). The SCF computation yields bond orders which are used to scale the bond stretching force constants, standard bond lengths and twofold torsional barriers.*

The following is a step-wise overview of the process:

1. A Fock matrix is generated based on the favorability of electron sharing between pairs of atoms in a pi system.
2. The pi molecular orbitals are computed from the Fock matrix.
3. The pi molecular orbitals are used to compute a new Fock matrix, then this new Fock matrix is used to compute better pi molecular orbitals.

   Step 2 and 3 are repeated until the computation of the Fock matrix and the pi molecular orbitals converge. This method is called the self-consistent field technique or a pi-SCF calculation.
4. A pi bond order is computed from the pi molecular orbitals.
5. The pi bond order is used to modify the bond length(BL_{res}) and force constant (K_{sres}) for each bond in the pi system.

6. The modified values of K_{sres} and BL_{res} are used in the molecular mechanics portion of the MM2 computation to further refine the molecule.

Stretch-Bend Cross Terms

Stretch-bend cross terms are used when a coupling occurs between bond stretching and angle bending. For example, when an angle is compressed, the MM2 force field uses the stretch-bend force constants to lengthen the bonds from the central atom in the angle to the other two atoms in the angle.

The force constant (K_{sb}) differs for different atom combinations.

The seven different atom combinations where force constants are available for describing the situation follow:

- X-B, C, N, O-Y
- B-B, C, N, O-H
- X-Al, S-Y
- X-Al, S-H
- X-Si, P-Y
- X-Si, P-H
- X-Ga, Ge, As, Se-Y, P-Y

where X and Y are any non-hydrogen atom.

User-Imposed Constraints

Additional terms are included in the force field when constraints are applied to torsional angles and non-bonded distances by the Optimal field in the Measurements table. These terms use a harmonic potential function, where the force constant has been set to a large value (4 for torsional constraints and 10^6 for non-bonded distances) in order to enforce the constraint.

For torsional constraints the additional term and force constant is described by:

For non-bonded distance constraints the additional term and force constant is:

Molecular Dynamics Simulation

In its broadest sense, molecular dynamics is concerned with simulating molecular motion. Motion is inherent to all chemical processes. Simple vibrations, like bond stretching and angle bending, give rise to IR spectra. Chemical reactions, hormone-receptor binding, and other complex processes are associated with many kinds of intramolecular and intermolecular motions. The MM2 method of molecular dynamics simulation uses Newton's equations of motion to simulate the movement of atoms.

Conformational transitions and local vibrations are the usual subjects of molecular dynamics studies. Molecular dynamics alters the values of the intramolecular degrees of freedom in a stepwise fashion. The steps in a molecular dynamics simulation represent the changes in atom position over time, for a given amount of kinetic energy.

The driving force for chemical processes is described by thermodynamics. The mechanism by which chemical processes occur is described by kinetics. Thermodynamics describes the energetic relationships between different chemical states, whereas the sequence or rate of events that occur as molecules transform between their various possible states is described by kinetics.

The Molecular Dynamics (MM2) command in the Calculations menu can be used to compute a molecular dynamics trajectory for a molecule or fragment in Chem3D. A common use of molecular dynamics is to explore the conformational space accessible to a molecule, and to prepare sequences of frames representing a molecule in motion. For more information on Molecular Dynamics see Chapter 9, "MM2 and MM3 Computations" on page 151.

Molecular Dynamics Formulas

The molecular dynamics computation consists of a series of steps that occur at a fixed interval, typically about 2.0 fs (femtoseconds, 1.0 x 10^{-15} seconds). The Beeman algorithm for integrating the equations of motion, with improved coefficients (B. R. Brooks) is used to compute new positions and velocities of each atom at each step.

Each atom (i) is moved according to the following formula:

$$x_i = x_i + v_i\Delta t + (5a_i - a_i^{old})\ (\Delta t)^2/8$$

Similarly, each atom is moved for y and z, where x_i, y_i, and z_i are the Cartesian coordinates of the atom, v_i is the velocity, a_i is the acceleration, a_i^{old} is the acceleration in the previous step, and Δt is the time between the current step and the previous step. The potential energy and derivatives of potential energy (g_i) are then computed with respect to the new Cartesian coordinates.

New accelerations and velocities are computed at each step according to the following formulas (m_i is the mass of the atom):

$$a_i^{veryold} = a_i^{old}$$

$$a_i^{old} = a_i$$

$$a_i = -g_i / m_i$$

$$v_i = v_i + (3a_i + 6a_i^{old} - a_i^{veryold})\ \Delta t / 8$$

Quantum Mechanics Theory in Brief

The following information is intended to familiarize you with the terminology of quantum mechanics and to point out the areas where approximations are made in semiempirical and ab initio methods. For complete derivations of equations used in quantum mechanics, you can refer to any quantum chemistry text book.

Quantum mechanical methods describe molecules in terms of explicit interactions between electrons and nuclei. Both ab initio and semiempirical methods are based on the following principles:

- Nuclei and electrons are distinguished from each other.
- Electron-electron (usually averaged) and electron-nuclear interactions are explicit.
- Interactions are governed by nuclear and electron charges (i.e. potential energy) and electron motions.
- Interactions determine the spatial distribution of nuclei and electrons and their energies.
- Quantum mechanical methods are concerned with approximate solutions to Schrödinger's wave equation.

$$H\Psi = E\Psi$$

- The Hamiltonian operator, H, contains information describing the electrons and nuclei in a system. The electronic wave function, Ψ, describes the state of the electrons in terms of their motion and position. E is the energy associated with the particular state of the electron.

NOTE: *The Schrödinger equation is an eigenequation, where the "H" operator, the Hamiltonian, operates on the wave function to return*

the same wave function and a constant. The wave function is called an eigenfunction, and the constant, an eigenvalue.

- Exact solutions to the Schrödinger equation are possible only for the simplest 1 electron-1 nucleus system. These solutions, however, yield the basis for all of quantum mechanics.
- The solutions describe a set of allowable states for an electron. The observable quantity for these states is described as a probability function. This function is the square of the wave function, and when properly normalized, describes the probability of finding an electron in that state.

$$\int \Psi^2(r)dr = 1$$

where r = radius (x, y, and z)

- There are many solutions to this probability function. These solutions are called atomic orbitals, and their energies, orbital energies.
- For a molecule with many electrons and nuclei the aim is to be able to describe molecular orbitals and energies in as analogous a fashion to the original Schrödinger equation as possible.

Approximations to the Hamiltonian

The first approximation made is known as the Born-Oppenheimer approximation, which allows separate treatment of the electronic and nuclear energies. Due to the large mass difference between an electron and a nucleus, a nucleus moves so much more slowly than an electron that it can be regarded as motionless relative to the electron. In effect, this approximation considers electrons to be moving with respect to a fixed nucleus. This allows the electronic energy to be described separately from nuclear energy by an electronic Hamiltonian, which can be solved at any set of nuclear coordinates. The electronic version of the Schrödinger equation is:

Another approximation assumes that electrons act independently of one another, or, more accurately, that each electron is influenced by an average field created by all other electrons and nuclei. Each electron in its own orbital is unimpeded by its neighbors.

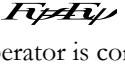
The electronic Hamiltonian is thus simplified by representing it as a sum of 1-electron Hamiltonians, and the wave equation becomes solvable for individual electrons in a molecule once a functional form of the wave function can be derived.

$$H_{elec} = \sum_i H_i^{eff}$$

$$H^{eff}\psi = \varepsilon\psi$$

For a molecular system, a matrix of these 1-electron Hamiltonians is constructed to describe the 1-electron interactions between a single electron and the core nucleus. The following represents the matrix for two atomic orbitals, ϕ_μ and ϕ_ν.

However, in molecular systems, this Hamiltonian does not account for the interaction between electrons with 2 or more different interaction centers or the interaction of two electrons. Thus, the Hamiltonian is further modified. This modification renames the Hamiltonian operator to the Fock operator.



The Fock operator is composed of a set of 1-electron Hamiltonians that describe the 1-electron, 1 center interactions and is supplemented by terms

that describe the interaction between 2-electrons. These terms include a density matrix, P, and the Coulomb and exchange integrals. The final equation for the Fock operator is represented by the Fock matrix.

The Fock matrix has two forms:

Restricted (RHF)— Requires that spin up and spin down electrons have the same energy and occupy the same orbital. U

Unrestricted (UHF)—Allows the alpha and beta spin electrons to occupy different orbitals and have different energies.

Restrictions on the Wave Function

For a molecular orbital (MO) with many electrons, the electronic wave function (Ψ) is restricted to meeting these requirements:

- Ψ must be normalized so that

$$\int_{-\infty}^{+\infty} |c\psi|^2 d\nu = n$$

  where n is the number of electrons. c is a normalization coefficient and Ψ^2 is interpreted as the probability density. This ensures that each electron exists somewhere in infinite space.
- Ψ must be antisymmetric, meaning that it must change sign if the positions of the electrons in a doubly-occupied MO are switched. This requirement accommodates the Pauli exclusion principle.

Spin functions

Spin functions, α and β, represent the allowed angular momentum states for each electron, spin up ($\uparrow$) and spin down ($\downarrow$) respectively. The product of the spatial function (ϕ_I), which represents the MO, and the spin function is the spin orbital ($\alpha\phi_i$ or $\beta\phi_I$ are the only two possible for any single MO). Spin orbitals are orthogonal.

LCAO and Basis Sets

Rigorous solution of the Hartree-Fock equations, while possible for atoms, is not possible for molecules. Generally an approximation known as Linear Combination of Atomic Orbitals (LCAO) must be used to compute MOs. This uses the sum of 1-electron atomic orbitals whose individual contributions to the MO is each weighted by a molecular orbital expansion coefficient, C_{vi}.

$$\psi_i = \sum_\nu C_{\nu i}\phi_\nu$$

The set of atomic orbitals, $\{\phi_\nu\}$, being used to generate the sum is called the basis set. Choice of an appropriate basis set $\{\phi_\nu\}$ is an important consideration in *ab initio* methods.

There are a number of functions and approaches used to derive basis sets. Basis sets are generally composed of linear combinations of Gaussian functions designed to approximate the AOs.

Minimal basis sets, such as STO-3G, contain one contracted Gaussian function (single zeta) for each occupied AO, while multiple-zeta basis sets (also called split valence basis sets) contain two or more contracted Gaussian functions. For example, a double-zeta basis set, such as the Dunning-Huzinaga basis set (D95), contains twice as many basis functions as the minimal one, and a triple-zeta basis set, such as 6-311G, contains three times as many basis functions.

Polarized basis sets allow AOs to change shape for angular momentum values higher than ground-state configurations by using polarization functions. The 6-31G* basis set, for example, adds d functions to heavy atoms.

A variety of other basis sets, such as diffuse function basis sets and high angular momentum basis sets, are tailored to the properties of particular of models under investigation.

The coefficients ($C_{\nu i}$) used for a given AO basis set (ϕ_ν) are derived from the solution of the Roothaan-Hall matrix equation with a diagonalized matrix of orbital energies, E.

The Roothaan-Hall Matrix Equation

This equation, shown below, includes the Fock matrix (F), the matrix of molecular orbital coefficients (C) from the LCAO approximation, the overlap matrix (S), and the diagonalized molecular orbital energies matrix (E).

$$FSCE$$

Since the Fock equations are a function of the molecular orbitals, they are not linearly independent. As such the equations must be solved using iterative, self-consistent field (SCF) methods. The initial elements in the Fock matrix are guessed. The molecular coefficients are calculated and the energy determined. Each subsequent iteration uses the results of the previous iteration until no further variation in the energy occurs (a self-consistent field is reached).

Ab Initio vs. Semiempirical

Ab initio (meaning literally "from first principles") methods use the complete form of the Fock operator to construct the wave equation. The semiempirical methods use simplified Fock operators, in which 1-electron matrix elements and some of the two electron integral terms are replaced by empirically determined parameters.

Both the SCF RHF and UHF methods underestimate the electron-electron repulsion and lead to electron correlation errors, which tend to overestimate the energy of a model. The use of configuration interaction (CI) is one method available to correct for this overestimation. For more information see "Configuration Interaction" on page 147.

The Semi-empirical Methods

Semiempirical methods can be divided into two categories: one-electron types and two-electron types. One-electron semiempirical methods use only a one-electron Hamiltonian, while two-electron methods use a Hamiltonian which includes a two-electron repulsion term. Authors differ concerning the classification of methods with one-electron Hamiltonians; some prefer to classify these as empirical.

The method descriptions that follow represent a very simplified view of the semiempirical methods available in Chem3D and CS MOPAC. For more information see the online MOPAC manual.

Extended Hückel Method

Developed from the qualitative Hückel MO method, the Extended Hückel Method (EH) represents the earliest one-electron semiempirical method to incorporate both σ and p valence systems. It is still widely used, owing to its versatility and success in analyzing and interpreting ground-state properties of organic, organometallic, and inorganic compounds of biological interest. Built into Chem3D, EH is the default semiempirical method used to calculate data required for displaying molecular surfaces.

The EH method uses a one-electron Hamiltonian with matrix elements defined as follows:

$$H_{\mu\mu} = -I_\mu$$

$$H_{\mu\nu} = 0.5K(H_{\mu\mu} + H_{\nu\nu})S_{\mu\nu} \qquad \mu \neq \nu$$

where I_μ is the valence state ionization energy (VSIE) of orbital μ as deduced from spectroscopic data, and K is the Wolfsberg-Helmholtz constant

(usually taken as 1.75). The Hamiltonian neglects electron repulsion matrix elements but retains the overlap integrals calculated using Slater-type basis orbitals. Because the approximated Hamiltonian (H) does not depend on the MO expansion coefficient C_{vi}, the matrix form of the EH equations:

$$HSCE$$

can be solved without the iterative SCF procedure.

Methods Available in CS MOPAC

The approximations that MOPAC uses in solving the matrix equations for a molecular system follow. Some areas requiring user choices are:

- RHF or UHF methods
- Configuration Interaction (CI)
- Choice of Hamiltonian approximation (potential energy function)

RHF

The default Hartree-Fock method assumes that the molecule is a closed shell and imposes spin restrictions. The spin restrictions allow the Fock matrix to be simplified. Since alpha (spin up) and beta (spin down) electrons are always paired, the basic RHF method is restricted to even electron closed shell systems.

Further approximations are made to the RHF method when an open shell system is presented. This approximation has been termed the 1/2 electron approximation by Dewar. In this method, unpaired electrons are treated as two 1/2 electrons of equal charge and opposite spin. This allows the computation to be performed as a closed shell. A CI calculation is automatically invoked to correct errors in energy values inherent to the 1/2 electron approximation. For more information see "Configuration Interaction" on page 147.

With the addition of the 1/2 electron approximation, RHF methods can be run on any starting configuration.

UHF

The UHF method treats alpha (spin up) and beta (spin down) electrons separately, allowing them to occupy different molecular orbitals and thus have different orbital energies. For many open and closed shell systems, this treatment of electrons results in better estimates of the energy in systems where energy levels are closely spaced, and where bond breaking is occurring.

UHF can be run on both open and closed shell systems. The major caveat to this method is the time involved. Since alpha and beta electrons are treated separately, twice as many integrals need to be solved. As your models get large, the time for the computation may make it a less satisfactory method.

Configuration Interaction

The effects of electron-electron repulsion are underestimated by SCF-RHF methods, which results in the overestimation of energies.

SCF-RHF calculations use a single determinant that includes only the electron configuration that describes the occupied orbitals for most molecules in their ground state. Further, each electron is assumed to exist in the average field created by all other electrons in the system, which tends to overestimate the repulsion between electrons. Repulsive interactions can be minimized by allowing the electrons to exist in more places (i.e. more orbitals, specifically termed virtual orbitals). The multi-electron configuration interaction (MECI) method in MOPAC addresses this problem by allowing multiple sets of electron assignments (i.e., configurations) to be used in constructing the molecular wave functions.

Molecular wave functions representing different configurations are combined in a manner analogous to the LCAO approach.

For a particular molecule, configuration interaction uses these occupied orbitals as a reference electron configuration and then promotes the electrons to unoccupied (virtual) orbitals. These new states, Slater determinants or microstates in MOPAC, are then linearly combined with the ground state configuration. The linear combination of microstates yields an improved electronic configuration and hence a better representation of the molecule.

Approximate Hamiltonians in MOPAC

There are five approximation methods available in MOPAC:

- AM1
- MNDO
- MNDO-d
- MINDO/3
- PM3

The potential energy functions modify the HF equations by approximating and parameterizing aspects of the Fock matrix.

The approximations in semiempirical MOPAC methods play a role in the following areas of the Fock operator:

- The basis set used in constructing the 1-electron atom orbitals is a minimum basis set of only the s and p Slater Type Orbitals (STOs) for valence electrons.
- The core electrons are not explicitly treated. Instead they are added to the nucleus. The nuclear charge is termed $N_{effective}$. For example, Carbon as a nuclear charge of +6-2 core electrons for a effective nuclear charge of +4.
- Many of the 2-electron Coulomb and Exchange integrals are parameterized based on element.

Choosing a Hamiltonian

Overall, these potential energy functions may be viewed as a chronological progression of improvements from the oldest method, MINDO/3 to the newest method, PM3. However, although the improvements in each method were designed to make global improvements, they have been found to be limited in certain situations.

The two major questions to consider when choosing a potential function are:

- Is the method parameterized for the elements in the model?
- Does the approximation have limitations which render it inappropriate for the model being studied?

For more detailed information see the MOPAC online manual.

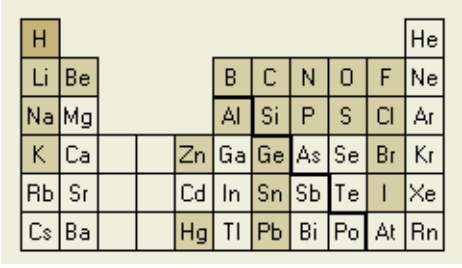
MINDO/3 Applicability and Limitations

MINDO/3 (Modified Intermediate Neglect of Diatomic Overlap revision 3) is the oldest method. Using diatomic pairs, it is an INDO (Intermediate Neglect of Diatomic Orbitals) method, where the degree of approximation is more severe than the NDDO methods MNDO, PM3 and AM1. This method is generally regarded to be of historical interest only, although some sulfur compounds are still more accurately analyzed using this method.

The following table shows the diatomic pairs that are parameterized in MINDO/3. An x indicates parameter availability for the pair indicated by the row and column. Parameters of dubious quality are indicated by (x).

	H	B	C	N	O	F	Si	P	S	Cl
H	x									
B	(x)	(x)								
C	x	(x)	x							
N	x	(x)	x	x						
O	x	(x)	x	x	x					
F	x	(x)	x	x	x	x				
Si	x		x				x			
P	x		x					x		
S	x		x	x	x	x			x	
Cl	x		x	x	x			x	x	x

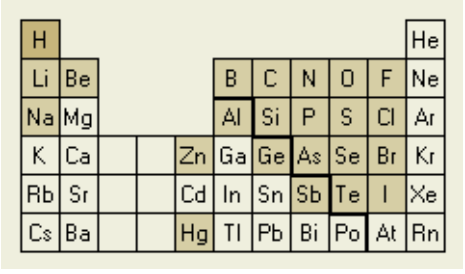
MNDO Applicability and Limitations



The following limitations apply to MNDO:

- Sterically crowded molecules are too unstable, for example, neopentane.
- Four-membered rings are too stable, for example, cubane.
- Hydrogen bonds are virtually non-existent, for example, water dimer. Overly repulsive nonbonding interactions between hydrogens and other atoms are predicted. In particular, simple H-bonds are generally not predicted to exist using MNDO.
- Hypervalent compounds are too unstable, for example, sulfuric acid.
- Activation barriers are generally too high.
- Non-classical structures are predicted to be unstable relative to the classical structure, for example, ethyl radical.
- Oxygenated substituents on aromatic rings are out-of-plane, for example, nitrobenzene.
- The peroxide bond is systematically too short by about 0.17 Å.
- The C-O-C angle in ethers is too large.

AM1 Applicability and Limitations



Important factors relevant to AM1 are:

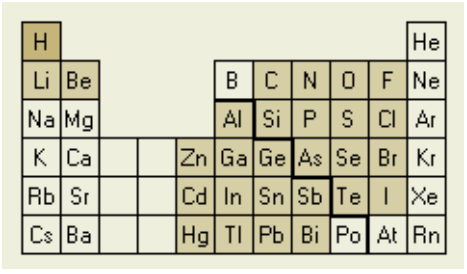
- AM1 is similar to MNDO; however, there are changes in the core-core repulsion terms and reparameterization.
- AM1 is a distinct improvement over MNDO, in that the overall accuracy is considerably improved. Specific improvements are:
  - The strength of the hydrogen bond in the water dimer is 5.5 kcal/mol, in accordance with experiment.
  - Activation barriers for reaction are markedly better than those of MNDO.
  - Hypervalent phosphorus compounds are considerably improved relative to MNDO.
  - In general, errors in ΔH_f obtained using AM1 are about 40% less than those given by MNDO.
  - AM1 phosphorus has a spurious and very sharp potential barrier at 3.0Å. The effect of this is to distort otherwise symmetric geometries and to introduce spurious

activation barriers. A vivid example is given by P_4O_6, in which the nominally equivalent P-P bonds are predicted by AM1 to differ by 0.4Å. This is by far the most severe limitation of AM1.

- Alkyl groups have a systematic error due to the heat of formation of the CH_2 fragment being too negative by about 2 kcal/mol.
- Nitro compounds, although considerably improved, are still systematically too positive in energy.
- The peroxide bond is still systematically too short by about 0.17Å.

PM3 Applicability and Limitations

PM3 (Parameterized Model revision 3) may be applied to the elements shaded in the following table:

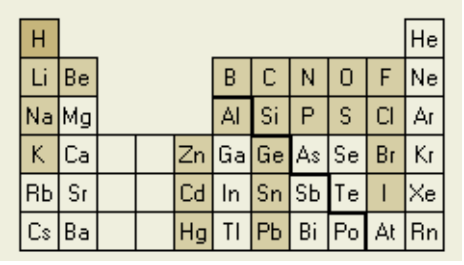


The following apply to PM3:

- PM3 is a reparameterization of AM1.
- PM3 is a distinct improvement over AM1.
- Hypervalent compounds are predicted with considerably improved accuracy.
- Overall errors in ΔH_f are reduced by about 40% relative to AM1.
- Little information exists regarding the limitations of PM3. This should be corrected naturally as results of PM3 calculations are reported.
- The barrier to rotation in formamide is practically non-existent. In part, this can be corrected by the use of the MMOK option. The MMOK option is used by default in CS MOPAC. For more information about MMOK see the online MOPAC Manual.

Ultra MNDO-d Applicability and Limitations

MNDO-d (Modified Neglect of Differential Overlap with d-Orbitals) may be applied to the elements shaded in the table below:



MNDO-d is a reformulation of MNDO with an extended basis set to include d-orbitals. This method may be applied to the elements shaded in the table below. Results obtained from MNDO-d are generally superior to those obtained from MNDO. The MNDO method should be used where it is necessary to compare or repeat calculations previously performed using MNDO.

The following types of calculations, as indicated by MOPAC keywords, are incompatible with MNDO-d:

- COSMO (Conductor-like Screening Model) solvation
- POLAR (polarizability calculation)
- GREENF (Green's Function)
- TOM (Miertus-Scirocco-Tomasi self-consistent reaction field model for solvation)

Chapter 9: MM2 and MM3 Computations

CS Mechanics Overview

The CS Mechanics add-in module for Chem3D provides three force-fields—MM2, MM3, and MM3 (Proteins)—and several optimizers that allow for more controlled molecular mechanics calculations. The default optimizer used is the Truncated-Newton-Raphson method, which provides a balance between speed and accuracy. Other methods are provided that are either fast and less accurate, or slow but more accurate.

The Chem3D atom types are translated to the atom types required for the calculations implemented in CS Mechanics. In some cases the translation is not quite correct since Chem3D has many more atom types than the standard MM2 and MM3 parameters, and also has the ability to guess missing types. In other cases the atom types are correctly defined, however the force field parameters may not be defined. This will result in calculations failing due to missing atom types or parameters. This problem can be resolved either by adding the missing parameters using the Additional Keywords section of the CS Mechanics interface, or by creating an input file which can be corrected with a text editor. The calculation can then be run by using the **Run Input** command in the Mechanics submenu of the **Calculations** menu. Further details on how to define missing parameters can be found in the Tinker manual (Tinker.pdf) on the ChemOffice CDROM.

The behavior of the user interface closely matches that of the other add-in modules such as MOPAC and Gaussian. The calculations can be set-up by making selections of force-field, termination criteria etc. Various properties can be computed as part of the single point or geometry optimization calculations. These can be selected from the Properties panel.

The Chem3D **MM2** submenu of the **Calculations** menu provides computations using the MM2 force field.

The MM2 procedures described assume that you understand how the potential energy surface relates to conformations of your model. If you are not familiar with these concepts, see 'Computation Concepts"

As discussed in , the energy minimization routine performs a local minimization only. Therefore, the results of minimization may vary depending on the starting conformation in a model.

Minimize Energy

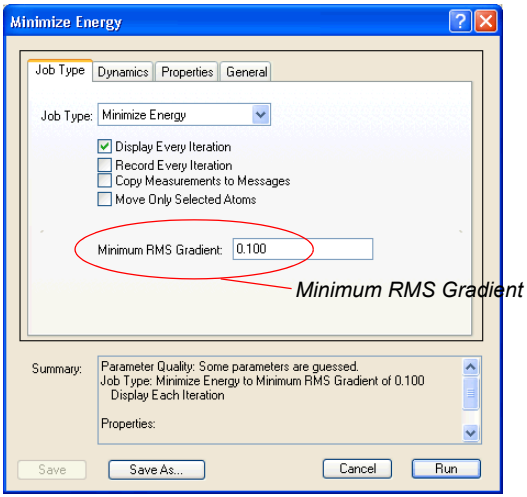
To minimize the energy of the molecule based on MM2 Force Field:

NOTE: *You cannot minimize models containing phosphate groups drawn with double bonds. For information on how to create a model with phosphate groups you can minimize, see the Chem3D Drawing FAQ at:*
http://www.cambridgesoft.com/services/faqs.cfm

1. Build the model for which you want to minimize the energy.
2. To impose constraints on model measurements, set **Optimal** column measurements in the Measurements table.

3. From the **Calculations** menu, point to **MM2**, and choose **Minimize Energy**.

   The Minimize Energy dialog box appears.



4. Set the convergence criteria using the following options:.

If you want to ...	Then ...
specify the convergence criteria for the gradient of the potential energy surface	Enter a value for **Minimum RMS Gradient**. If the slope of the potential energy surface becomes too small, then the minimization has probably reached a local minimum on the potential energy surface, and the minimization terminates. The default value of 0.100 is a reasonable compromise between accuracy and speed. Reducing the value means that the calculation continues longer as it tries to get even closer to a minimum. Increasing the value shortens the calculation, but leaves you farther from a minimum. Increase the value if you want a better optimization of a conformation that you know is not a minimum, but you want to isolate for computing comparative data.
watch the minimization process "live" at each iteration in the calculation	Select **Display Every Iteration**. *NOTE: Displaying or recording each iteration adds significantly to the time required to minimize the structure.*

If you want to ...	Then ...
store each iteration as a frame in a movie for replay later	Select **Record Every Iteration**.
view the value of each measurement in the Output window	Select **Copy Measurements to Output**.
restrict movement of a selected part of a model during the minimization	Select **Move Only Selected Atoms**. Constraint is not imposed on any term in the calculation and the values of any results are not affected.

NOTE: *If you are planning to make changes to any of the MM2 constants, such as cutoff values or other parameters used in the MM2 force field, please make a backup copy of the parameter tables before making any changes. This will assure that you can get back the values that are shipped with Chem3D, in case you need them*

NOTE: *Chem3D guesses parameters if you try to minimize a structure containing atom types not supported by MM2. Examples include inorganic complexes where known parameters are limited. You can view all parameters used in the analysis using the Show Used Parameters command. See* *"Showing Used Parameters" on page 163*.

Running a Minimization

To begin the minimization of a model:

- Click **Run**.

  TIP: *In all of the following minimization examples, you can use the MM2 icon on the Calculation toolbar instead of the Calculations menu.*

  The Output window appears when the minimization begins, if it was not already opened. The data is updated for every iteration of the computation, showing the iteration number, the steric energy value at that iteration, and the RMS gradient. If you have not selected the **Copy Measurements to Output** option, only the last iteration is displayed.

  After the RMS gradient is reduced below the requested value, the minimization ends, and the final steric energy components and total appear in the Output window.

  Intermediate status messages may appear in the Output window. A message appears if the minimization terminates abnormally, usually due to a poor starting conformation.

To interrupt a minimization that is in progress:

- Click **Stop** in the **Computing** dialog box.

  The minimization and recording stops.

Queuing Minimizations

You can start to minimize several models without waiting for each model to finish minimizing. If a computation is in progress when you begin

minimizing a second model, the minimization of the second model is delayed until the first minimization stops.

If you are using other applications, you can run minimization with Chem3D in the background. You can perform any action in Chem3D that does not change the position of an atom or add or delete any part of the model. For example, you can move windows around during minimization, change settings, or scale your model.

Minimizing Ethane

Ethane is a particularly straightforward example of minimization, because it has only one minimum-energy (staggered) and one maximum-energy (eclipsed) conformation.

To minimize energy in ethane:

1. From the **File** menu, choose **New**.

   An empty model window appears.
2. Click the Single Bond tool.
3. Drag in the model window.

   A model of Ethane appears.
4. Choose **Show Serial Numbers** on the **Model Display** submenu of the **View** menu.

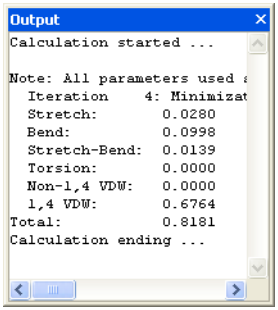
   You might also want to set the **Model Display Mode** to Ball and Stick or Cylindrical Bonds.
5. On the **Calculations** menu, point to **MM2** and choose **Minimize Energy**.
6. Click **Run** on the Minimize Energy dialog box.

   The calculation is performed. Messages appear in the Output Window.

To view all the messages:

- Scroll in the Output Window.

You can also "tear off" the window and enlarge it to make it easier to view.

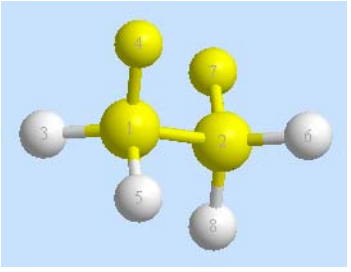


The Total Steric Energy for the conformation is 0.8181 kcal/mol. The 1,4 VDW term of 0.6764 dominates the steric energy. This term is due to the H-H repulsion contribution.

NOTE: *The values of the energy terms shown are approximate and can vary slightly based on the type of processor used to calculate them.*

To view the value of one of the dihedral angles that contributes to the 1,4 VDW contribution:

1. Select the atoms making up the dihedral angle as shown below by Shift+clicking **H(7)**, **C(2)**, **C(1)**, and **H(4)** in that order.



2. From the **Structure** menu, point to **Measurement**, and select **Set Dihedral Measurement**.

The following measurement appears.

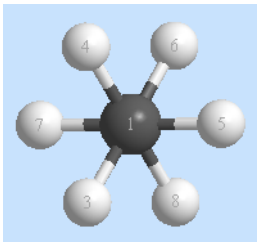
Measurement

	Atoms	Actual	Optimal
1	H(4)-C(1)-C(2)-H(7)	-59.9441	

The 60 degree dihedral represents the lowest energy conformation for the ethane model.

Select the Trackball tool:

1. Reorient the model by dragging the X- and Y-axis rotation bars until you have an end-on view.

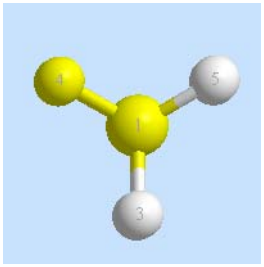


To force a minimization to converge on the transition conformation, set the barrier to rotation:

1. In the **Measurements** table, type 0 in the **Optimal** column for the selected dihedral angle and press the **Enter** key.
2. On the MM2 submenu of the **Calculations** menu, choose **Minimize**.

   The Minimize Energy dialog box appears.
3. Click **Run**.

   The model conforms to the following structure:



Entering a value in the **Optimal** column imposes a constraint on the minimization routine. You are increasing the force constant for the torsional term in the steric energy calculation so that you can optimize to the transition state.

When the minimization is complete, the reported energy values are as follows. The energy for this eclipsed conformation is higher relative to the staggered form. The majority of the energy contribution is from the torsional energy and the 1,4 VDW interactions.

NOTE: *The values of the energy terms shown here are approximate and can vary slightly based on the type of processor used to calculate them.*

Output

```
Calculation started ...

Note: All parameters used
  Iteration  196: Minimizat
  Stretch:        0.0420
  Bend:           0.2009
  Stretch-Bend:   0.0242
  Torsion:        2.1328
  Non-1,4 VDW:    0.0000
  1,4 VDW:        1.1527
Total:            3.5526
Calculation ending ...
```

The dihedral angle in the Actual column becomes 0, corresponding to the imposed constraint.

The difference in energy between the global minimum (Total, previous calculation) and the transition state (Total, this calculation) is 2.73 kcal/mole, which is in agreement with literature values.

To further illustrate points about minimization:

- Delete the value from the **Optimal** column for the dihedral angle and click the MM2 icon on the Calculation toolbar.

After the minimization is complete, you are still at 0 degrees. This is an important consideration for working with the MM2 minimizer. It uses first derivatives of energy to determine the next logical

move to lower the energy. However, for saddle points (transition states), the region is fairly flat and the minimizer is satisfied that a minimum is reached. If you suspect your starting point is not a minimum, try setting the dihedral angle off by about 2 degrees and minimize again.

Comparing Two Stable Conformations of Cyclohexane

In the following example you compare the cyclohexane twist-boat conformation and the chair global minimum.

To build a model of cyclohexane:

1. From the **File** menu, choose **New**.

   An empty model window appears.
2. Select the Text Building tool.
3. Click in the model window.

   A text box appears.
4. Type CH2(CH2)5 and press the **Enter** key.

CAUTION

While there are other, perhaps easier, methods of creating a cyclohexane model, you should use the method described to follow this example.

Before minimizing, it is wise to use the **Clean Up Structure** command to refine the model. This generally improves the ability of the Minimize Energy command to reach a minimum point.

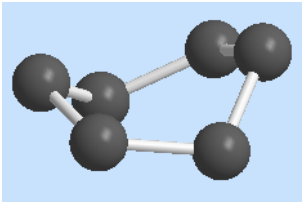
1. From the **Edit** menu, choose **Select All**.
2. From the **Structure** menu, choose **Clean Up**.

NOTE: *The Clean Up command is very similar to the minimize energy command in that it is a preset, short minimization of the structure.*

To perform the minimization:

- From the **MM2** submenu of the **Calculations** menu, choose **Minimize Energy**, and click **Run**.

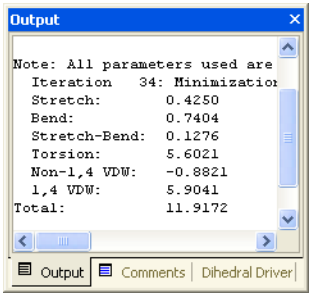
  When the minimization is complete, reorient the model so it appears as follows.



The conformation you converged to is not the well-known chair conformation, which is the global minimum. Instead, the model has converged on a local minimum, the twisted-boat conformation. This is the closest low-energy conformation to your starting conformation.

Had you built this structure using substructures that are already energy minimized, or the ChemDraw panel, you would be close to the chair conformation. The minimizer does not surmount the saddle point to locate the global minimum, and the closest minimum is sought.

The energy values in the Output window should be approximately as follows:



The major contributions are from the 1,4 VDW and Torsional aspects of the model.

For cyclohexane, there are six equivalent local minima (twisted-boat), two equivalent global minima (chair), and many transition states (one of which is the boat conformation).

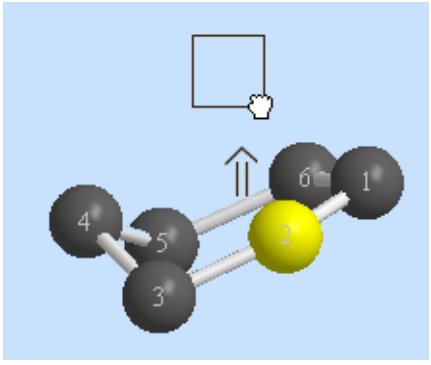
Locating the Global Minimum

Finding the global minimum is extremely challenging for all but the most simple molecules. It requires a starting conformation which is already in the valley of the *global* minimum, not in a *local* minimum valley. The case of cyclohexane is straightforward because you already know that the global minimum is either of the two possible chair conformations. To obtain the new starting conformation, change the dihedrals of the twisted conformation so that they represent the potential energy valley of the chair conformation.

The most precise way to alter a dihedral angle is to change its Actual value in the Measurements table when dihedral angles are displayed. An easier way to alter an angle, especially when dealing with a ring, is to move the atoms by dragging and then cleaning up the resulting conformation.

To change a dihedral angle:

- Drag C1 below the plane of the ring, then drag C4 above the plane of the ring.



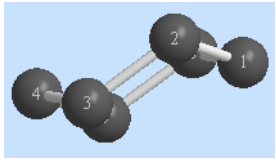
During dragging, the bond lengths and angles were deformed. To return them to the optimal values before minimizing:

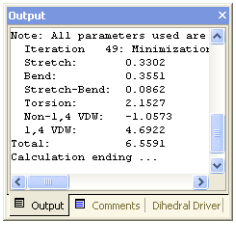
1. Select all (Ctrl+A) and run Clean Up.

Now run the minimization:

2. From the **MM2** submenu of the **Calculations** menu, choose **Minimize Energy** and click **Run**.
3. When the minimization is complete, reorient the model using the Rotation bars to see the final chair conformation.

NOTE: *The values of the energy terms shown here are approximate and can vary slightly based on the type of processor used to calculate them.*





This conformation is about 5.5 kcal/mole more stable than the twisted-boat conformation.

For molecules more complicated than cyclohexane, where you don't already know what the global minimum is, some other method is necessary for locating likely starting geometries for minimization. One way of accessing this conformational space of a molecule with large energy barriers is to perform molecular dynamics simulations. This, in effect, heats the molecule, thereby increasing the kinetic energy enough to surmount the energetically disfavored transition states.

Molecular Dynamics

Molecular Dynamics uses Newtonian mechanics to simulate motion of atoms, adding or subtracting kinetic energy as the model's temperature increases or decreases.

Molecular Dynamics allows you to access the conformational space available to a model by storing iterations of the molecular dynamics run and later examining each frame.

Performing a Molecular Dynamics Computation

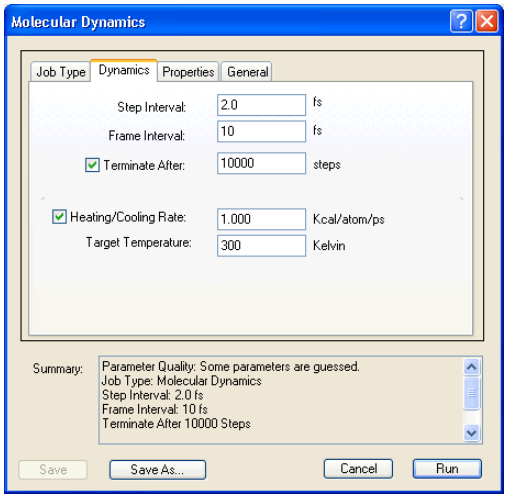
To perform a molecular dynamics simulation:

1. Build the model (or fragments) that you want to include in the computation.

   NOTE: *The model display type you use affects the speed of the molecular dynamics computation. Model display will decrease the speed in the following order: Wire Frame< Sticks < Ball and Sticks< Cylindrical Bonds < Ribbons< Space Fill and VDW dot surfaces < Molecular Surfaces.*

2. Minimize the energy of the model (or fragments), using MM2 or MOPAC.
3. To track a particular measurement during the simulation, choose one of the following:
   - Select the appropriate atoms, and choose **Set Bond Angle** or **Set Bond Length** on the **Measurement** submenu of the **Structure** menu.
4. Choose **Molecular Dynamics** on the **MM2** submenu of the **Calculations** menu of the **Calculations** menu.

   The Molecular Dynamics dialog box appears with the default values.



5. Enter the appropriate values.
6. Click **Run**.

Dynamics Settings

Use the **Dynamics** tab to enter parameter values for the parameters that define the molecular dynamics calculations:

- **Step Interval**—determines the time between molecular dynamics steps. The step interval must be less than ~5% of the vibration period for the highest frequency normal mode, (10 fs for a 3336 cm^{-1} H–X stretching vibration). Normally a step interval of 1 or 2 fs yields reasonable results. Larger step intervals may cause the integration method to break down, because higher order moments of the position are neglected in the Beeman algorithm.
- **Frame Interval**—determines the interval at which frames and statistics are collected. A frame interval of 10 or 20 fs gives a fairly smooth sequence of frames, and a frame interval of 100 fs or more can be used to obtain samples of conformational space over a longer computation.

- **Terminate After**—causes the molecular dynamics run to stop after the specified number of steps. The total time of the run is the Step Interval times the number of steps.
- **Heating/Cooling Rate**—dictates whether temperature adjustments are made. If the Heating/Cooling Rate check box is checked, the Heating/Cooling Rate slider determines the rate at which energy is added to or removed from the model when it is far from the target temperature.

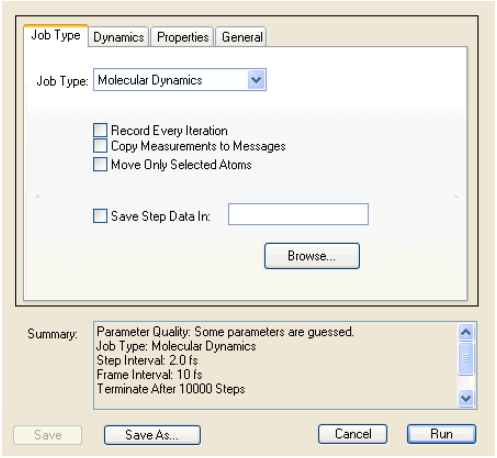
  A heating/cooling rate of approximately 1.0 kcal/atom/picosecond results in small corrections which minimally disturb the trajectory. A much higher rate quickly heats up the model, but an equilibration or stabilization period is required to yield statistically meaningful results.

  To compute an isoenthalpic trajectory (constant total energy), deselect **Heating/Cooling Rate**.
- **Target Temperature**—the final temperature to which the calculation will run. Energy is added to or removed from the model when the computed temperature varies more than 3% from the target temperature.

  The computed temperature used for this purpose is an exponentially weighted average temperature with a memory half-life of about 20 steps.

Job Type Settings

Use the **Job Type** tab to set options for the computation.



Select the appropriate options:

If you want to ...	Then Click ...
record each iteration as a frame in a movie for later replay	**Record Every Iteration**.
track a particular measurement	**Copy Measurements to Output**.
restrict movement of a selected part of a model during the minimization	**Move Only Selected Atoms**. Constraint is not imposed on any term in the calculation and the values of any results are not affected.

If you want to ...	Then Click ...
save a file containing the Time (in picoseconds), Total Energy, Potential Energy, and Temperature data for each step.	Click **Save Step Data In** and browse to choose a location for storing this file. The word "heating" or "cooling" appears for each step in which heating or cooling was performed. A summary of this data appears in the Message window each time a new frame is created.

To begin the computation:

- Click **Run**.

  The computation begins. Messages for each iteration and any measurements you are tracking appear in the Output window.

  If you have chosen to Record each iteration, the Movie menu commands (and Movie toolbar icons) will be active at the end of the computation.

The simulation ends when the number of steps specified is taken.

To stop the computation prematurely:

- Click **Stop** in the Computation dialog box.

Computing the Molecular Dynamics Trajectory for a Short Segment of Polytetrafluoroethylene (PTFE)

To build the model:

1. From the File menu, choose **New**.
2. Select the Text Building tool.
3. Click in the model window.

   A text box appears.
4. Type F(C2F4)6F and press the **Enter** key.

   A polymer segment consisting of six repeat units of tetrafluoroethylene appears in the model window.

To perform the computation:

1. Select C(2), the leftmost terminal carbon, then Shift+click C(33), the rightmost terminal carbon.
2. Choose **Set Distance** from the Measurement submenu of the Structure menu.

   A measurement for the overall length of the molecule appears in the Measurements table.
3. Choose **Molecular Dynamics** from the MM2 submenu of the Calculations menu.
4. Click the Job Type tab and click the checkbox for Copy Measurements to Output. If you want to save the calculation as a movie, select Record Every Iteration checkbox.
5. Click **Run**.

When the calculation begins, the Output Window appears.

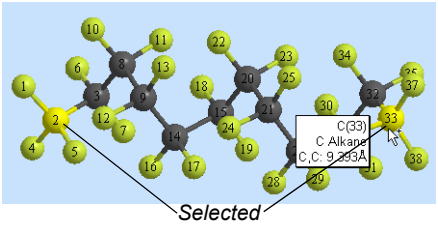
To replay the movie:

- Click **Start** on the Movie menu.

  The frames computed during the molecular dynamics calculation are played as a movie.

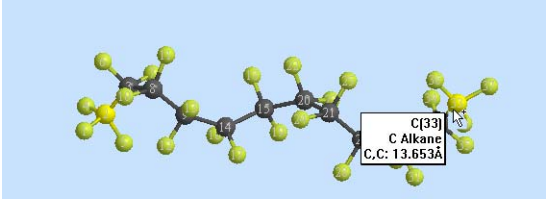
To review the results:

1. View the Output window to examine the measurement data included in the molecular dynamics step data.
2. Drag the **Movie slider knob** to the left until the first step appears.



The C(2)-C(33) distance for the molecule before the molecular dynamics calculation began is approximately 9.4Å.

3. Scroll down to the bottom of the Output window and examine the C(2)-C(33) distance for the molecule at 0.190 picoseconds (which corresponds to frame 20 in the Movie slider of the model window).



The C(2)-C(33) distance is approximately 13.7Å, 42% greater than the initial C(2)-C(33) distance.

Compute Properties

Compute Properties represents a single point energy computation that reports the total steric energy for the current conformation of a model (the active frame, if more than one exists).

NOTE: *The Steric Energy is computed at the end of an MM2 Energy minimization.*

A comparison of the steric energy of various conformations of a molecule gives you information on the relative stability of those conformations.

NOTE: *In cases where parameters are not available because the atom types in your model are not among the MM2 atom types supported, Chem3D will attempt an educated guess. You can view the guessed parameters by using the Show Used Parameters command after the analysis is completed.*

Compare the steric energies of *cis*- and *trans*-2-butene.

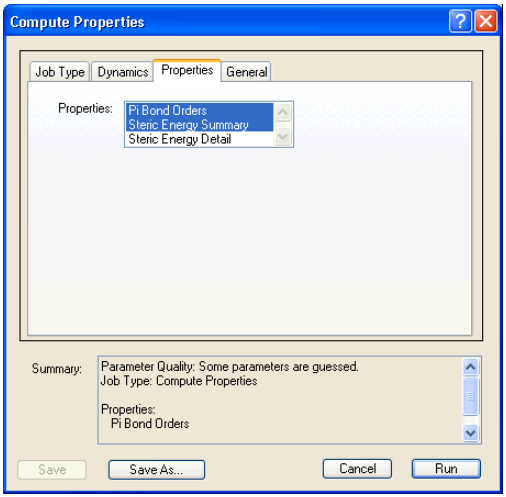
To build *trans*-2-butene and compute properties:

1. From the **File** menu, choose **New**.
2. Select the Text Building tool.
3. Click in the model window.

   A text box appears.
4. Type trans-2-butene and press the **Enter** key.

   A molecule of *trans*-2-butene appears in the model window.
5. From the **MM2** submenu of the **Calculations** menu, choose **Compute Properties**.

The Compute Properties dialog box appears.



6. Click **Run**.

   The Output window appears. When the steric energy calculation is complete, the individual steric energy terms and the total steric energy appear.

Use the Output window scroll bar to view all of the output. The units are kcal/mole for all terms. At the beginning of the computation the first message indicates that the parameters are of Quality=4 meaning that they are experimentally determined/verified parameters.

NOTE: *The values of the energy terms shown here are approximate and can vary slightly based on the type of processor used to calculate them.*

The following values are displayed:

- The Stretch term represents the energy associated with distorting bonds from their optimal length.
- The second steric energy term is the Bend term. This term represents the energy associated with deforming bond angles from their optimal values.
- The Stretch-Bend term represents the energy required to stretch the two bonds involved in a bond angle when that bond angle is severely compressed.
- The Torsion term represents the energy associated with deforming torsional angles in the molecule from their ideal values.
- The Non-1,4 van der Waals term represents the energy for the through-space interaction between pairs of atoms that are separated by more than three atoms.

For example, in *trans*-2-butene, the Non-1,4 van der Waals energy term includes the energy for the interaction of a hydrogen atom bonded to C(1) with a hydrogen atom bonded to C(4).

The 1,4 van der Waals term represents the energy for the through-space interaction of atoms separated by two atoms.

For example, in *trans*-2-butene, the 1,4 van der Waals energy term includes the energy for the interaction of a hydrogen atom bonded to C(1) with a hydrogen atom bonded to C(2).

The dipole/dipole steric energy represents the energy associated with the interaction of bond dipoles.

For example, in *trans*-2-butene, the Dipole/Dipole term includes the energy for the interaction of the two C Alkane/C Alkene bond dipoles.

To build a *cis*-2-butene and compute properties:

1. From the **Edit** menu, choose **Clear** to delete the model.
2. Double-click in the model window.

   A text box appears.
3. Type cis-2-butene and press the **Enter** key.

   A molecule of *cis*-2-butene appears in the model window.
4. From the **MM2** submenu of the **Calculations** menu, choose **Compute Properties**.

The steric energy terms for *cis*-2-butene appears in the Output window.

Below is a comparison of the steric energy components for *cis*-2-butene and *trans*-2-butene.

NOTE: *The values of the energy terms shown here are approximate and can vary slightly based on the type of processor used to calculate them.*

Energy Term	trans-2-butene	cis-2-butene
Stretch:	0.0627	0.0839
Bend:	0.2638	1.3235
Stretch-Bend:	0.0163	0.0435
Torsion:	-1.4369	-1.5366
Non-1,4 van der Waals:	-0.0193	0.3794
1,4 van der Waals:	1.1742	1.1621
Dipole/Dipole:	0.0767	0.1032
Total:	0.137	1.5512

The significant differences between the steric energy terms for *cis* and *trans*-2-butene are in the Bend and Non-1,4 van der Waals steric energy terms. The Bend term is much higher in *cis*-2-butene because the C(1)-C(2)-C(3) and the C(2)-C(3)-C(4) bond angles had to be deformed from their optimal value of 122.0° to 127.4° to relieve some of the steric crowding from the interaction of hydrogens on C(1) and C(4). The interaction of hydrogens on C(1) and C(4) of *trans*-2-butene is much less intense, thus the C(1)-C(2)-C(3) and the C(2)-C(3)-C(4) bond angles have values of 123.9°, much closer to the optimal value of 122.0°. The Bend and Non-1,4 van der Waals terms for *trans*-2-butene are smaller, therefore *trans*-2-butene has a lower steric energy than *cis*-2-butene.

Showing Used Parameters

You can display all parameters used in an MM2 calculation in the Output window. The list includes a quality assessment of each parameter. Highest quality empirically-derived parameters are rated as 4 while a lowest quality rating of 1 indicates that a parameter is a "best guess" value.

To show the used Parameters:

- From the MM2 submenu of the Calculations menu, choose **Show Used Parameters**.

  The parameters appear in the Output window.

Repeating an MM2 Computation

After you perform an MM2 computation, you can repeat the job as follows:

1. Choose **Repeat MM2 Job** from the MM2 submenu of the Calculations menu,

   The appropriate dialog box appears.
2. Change parameters if desired and click **Run**.

   The computation proceeds.

Using .jdf Files

The job type and settings are saved in a .jdf file if you click the **Save As** button on the dialog box before running a computation. You can then run these computations in a different work session.

To run a previously created MM2 job:

1. Choose **Run MM2 Job** from the MM2 submenu of the Calculations menu.
2. Choose the file and click **Open**.

   The dialog box for the appropriate computation appears.
3. Change parameters if desired and click **Run**.

Chapter 10: MOPAC Computations

Overview

MOPAC is a molecular computation application developed by Dr. James Stewart and supported by Fujitsu Corporation that features a number of widely-used, semi-empirical methods. It is available in two versions, Professional and Ultra.

MOPAC Pro allows you to compute properties and perform simple (and some advanced) energy minimizations, optimize to transition states, and compute properties. The CS MOPAC Pro implementation supports MOPAC sparkles, has an improved user interface, and provides faster calculations. It is included in some versions of Chem3D, or may be purchased as an optional addin.

MOPAC Ultra is the full MOPAC implementation, and is only available as an optional addin. The CS MOPAC Ultra implementation provides support for previously unavailable features such as MOZYME and PM5 methods.

In both cases, you need a separate installer to install the MOPAC application. Once installed, either version of MOPAC will work with either version of Chem3D.

NOTE: *If you have CS MOPAC installed on your computer from a previous Chem3D or ChemOffice installation, upgrading to version 9.0.1 will NOT remove your existing MOPAC installation. Chem3D will continue to support it, even if the update version does not include CS MOPAC. Installing either of the CS MOPAC 2002 versions will replace the existing MOPAC installation.*

CS MOPAC provides a graphical user interface that allows you to perform MOPAC computations directly on the model in the Chem3D model window. As a computation progresses, the model changes appearance to reflect the computed result.

In this section:

- A brief review of semi-empirical methods
- MOPAC Keywords used in CS MOPAC
- Electronic configuration (includes using MOPAC sparkles)
- Optimizing Geometry
- Using MOPAC Properties
- Using MOPAC files
- Computation procedures, with examples.
  - Minimizing Energy
  - Computing Properties
  - Optimizing to a Transition State
  - Computing Properties
- Examples
  - Locating the Eclipsed Transition State of Ethane
  - The Dipole Moment of Formaldehyde
  - Comparing Cation Stabilities in a Homologous Series of Molecules
  - Analyzing Charge Distribution in a Series Of Mono-substituted Phenoxy Ions
  - Calculating the Dipole Moment of meta-Nitrotoluene
  - Comparing the Stability of Glycine Zwitterion in Water and Gas Phase
  - Hyperfine Coupling Constants for the Ethyl Radical
  - RHF Spin Density for the Ethyl Radical

The procedures assume you have a basic understanding of the computational concepts and terminology of semi-empirical methods, and the concepts involved in geometry optimization (minimization) and single-point computations. For more information see "Computation Concepts" on page 129.

For help with MOPAC, see the online MOPAC manual at:
http://www.cachesoftware.com/mopac/Mopac2002manual/

MOPAC Semi-empirical Methods

The method descriptions that follow represent a very simplified view of the semi-empirical methods available in Chem3D and CS MOPAC. For more information see the online MOPAC manual.

Extended Hückel Method

Developed from the qualitative Hückel MO method, the Extended Hückel Method (EH) represents the earliest one-electron semi-empirical method to incorporate both σ and p valence systems. It is still widely used, owing to its versatility and success in analyzing and interpreting ground-state properties of organic, organometallic, and inorganic compounds of biological interest. Built into Chem3D, EH is the default semi-empirical method used to calculate data required for displaying molecular surfaces.

The EH method uses a one-electron Hamiltonian with matrix elements defined as follows:

$$H_{\mu\mu} = -I_{\mu}$$

$$H_{\mu\nu} = 0.5K(H_{\mu\mu} + H_{\nu\nu})S_{\mu\nu} \qquad \mu \neq \nu$$

where I_{μ} is the valence state ionization energy (VSIE) of orbital μ as deduced from spectroscopic data, and K is the Wolfsberg-Helmholtz constant (usually taken as 1.75). The Hamiltonian neglects electron repulsion matrix elements but retains the overlap integrals calculated using Slater-type basis orbitals. Because the approximated Hamiltonian (H) does not depend on the MO expansion coefficient $C_{\nu i}$, the matrix form of the EH equations:

$$HSCE$$

can be solved without the iterative SCF procedure.

RHF

The default Hartree-Fock method assumes that the molecule is a closed shell and imposes spin restrictions. The spin restrictions allow the Fock matrix to be simplified. Since alpha (spin up) and beta (spin down) electrons are always paired, the basic RHF method is restricted to even electron closed shell systems.

Further approximations are made to the RHF method when an open shell system is presented. This approximation has been termed the 1/2 electron approximation by Dewar. In this method, unpaired electrons are treated as two 1/2 electrons of equal charge and opposite spin. This allows the computation to be performed as a closed shell. A CI calculation is automatically invoked to correct errors in energy values inherent to the 1/2 electron approximation. For more information see "Configuration Interaction" on page 167.

With the addition of the 1/2 electron approximation, RHF methods can be run on any starting configuration.

UHF

The UHF method treats alpha (spin up) and beta (spin down) electrons separately, allowing them to occupy different molecular orbitals and thus have different orbital energies. For many open and closed shell systems, this treatment of electrons

results in better estimates of the energy in systems where energy levels are closely spaced, and where bond breaking is occurring.

UHF can be run on both open and closed shell systems. The major caveat to this method is the time involved. Since alpha and beta electrons are treated separately, twice as many integrals need to be solved. As your models get large, the time for the computation may make it a less satisfactory method.

Configuration Interaction

The effects of electron-electron repulsion are underestimated by SCF-RHF methods, which results in the overestimation of energies.

SCF-RHF calculations use a single determinant that includes only the electron configuration that describes the occupied orbitals for most molecules in their ground state. Further, each electron is assumed to exist in the average field created by all other electrons in the system, which tends to overestimate the repulsion between electrons. Repulsive interactions can be minimized by allowing the electrons to exist in more places (i.e. more orbitals, specifically termed virtual orbitals). The multi-electron configuration interaction (MECI) method in MOPAC addresses this problem by allowing multiple sets of electron assignments (i.e., configurations) to be used in constructing the molecular wave functions. Molecular wave functions representing different configurations are combined in a manner analogous to the LCAO approach.

For a particular molecule, configuration interaction uses these occupied orbitals as a reference electron configuration and then promotes the electrons to unoccupied (virtual) orbitals. These new states, Slater determinants or microstates in MOPAC, are then linearly combined with the ground state configuration. The linear combination of microstates yields an improved electronic configuration and hence a better representation of the molecule.

Approximate Hamiltonians in MOPAC

There are five approximation methods available in MOPAC:

- AM1
- MNDO
- MNDO-d
- MINDO/3
- PM3

The potential energy functions modify the HF equations by approximating and parameterizing aspects of the Fock matrix. The approximations in semi-empirical MOPAC methods play a role in the following areas of the Fock operator:

- The basis set used in constructing the 1-electron atom orbitals is a minimum basis set of only the s and p Slater Type Orbitals (STOs) for valence electrons.
- The core electrons are not explicitly treated. Instead they are added to the nucleus. The nuclear charge is termed $N_{effective}$.

  For example, Carbon as a nuclear charge of +6-2 core electrons for a effective nuclear charge of +4.
- Many of the 2-electron Coulomb and Exchange integrals are parameterized based on element.

Choosing a Hamiltonian

Overall, these potential energy functions may be viewed as a chronological progression of improvements from the oldest method, MINDO/3 to the newest method, PM5. However, although the

improvements in each method were designed to make global improvements, they have been found to be limited in certain situations.

The two major questions to consider when choosing a potential function are:

- Is the method parameterized for the elements in the model?
- Does the approximation have limitations which render it inappropriate for the model being studied?

For more detailed information see the MOPAC online manual.

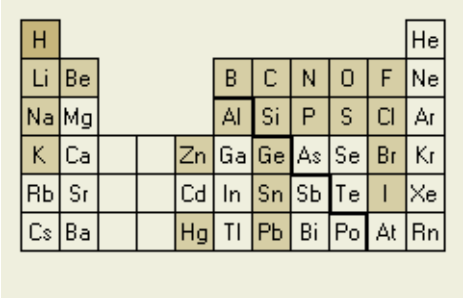
MINDO/3 Applicability and Limitations

MINDO/3 (Modified Intermediate Neglect of Diatomic Overlap revision 3) is the oldest method. Using diatomic pairs, it is an INDO (Intermediate Neglect of Diatomic Orbitals) method, where the degree of approximation is more severe than the NDDO methods MNDO, PM3 and AM1. This method is generally regarded to be of historical interest only, although some sulfur compounds are still more accurately analyzed using this method.

The following table shows the diatomic pairs that are parameterized in MINDO/3. An x indicates parameter availability for the pair indicated by the row and column. Parameters of dubious quality are indicated by (x).

	H	B	C	N	O	F	Si	P	S	Cl
H	x									
B	(x)	(x)								
C	x	(x)	x							
N	x	(x)	x	x						
O	x	(x)	x	x	x					
F	x	(x)	x	x	x	x				
Si	x		x				x			
P	x		x					x		
S	x		x	x	x	x			x	
Cl	x		x	x	x			x	x	x

MNDO Applicability and Limitations



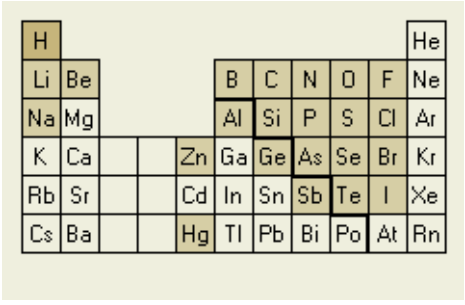
The following limitations apply to MNDO:

- Sterically crowded molecules are too unstable, for example, neopentane.
- Four-membered rings are too stable, for example, cubane.
- Hydrogen bonds are virtually non-existent, for example, water dimer. Overly repulsive nonbonding interactions between hydrogens

and other atoms are predicted. In particular, simple H-bonds are generally not predicted to exist using MNDO.

- Hypervalent compounds are too unstable, for example, sulfuric acid.
- Activation barriers are generally too high.
- Non-classical structures are predicted to be unstable relative to the classical structure, for example, ethyl radical.
- Oxygenated substituents on aromatic rings are out-of-plane, for example, nitrobenzene.
- The peroxide bond is systematically too short by about 0.17 Å.
- The C-O-C angle in ethers is too large.

AM1 Applicability and Limitations

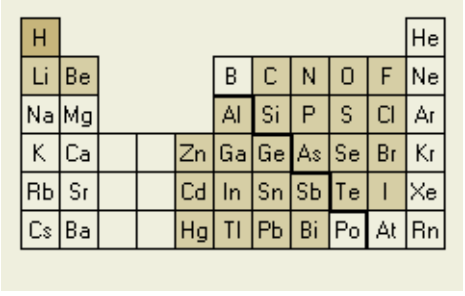


Important factors relevant to AM1 are:

- AM1 is similar to MNDO; however, there are changes in the core-core repulsion terms and reparameterization.
- AM1 is a distinct improvement over MNDO, in that the overall accuracy is considerably improved. Specific improvements are:
  - The strength of the hydrogen bond in the water dimer is 5.5 kcal/mol, in accordance with experiment.
  - Activation barriers for reaction are markedly better than those of MNDO.
  - Hypervalent phosphorus compounds are considerably improved relative to MNDO.
  - In general, errors in ΔH_f obtained using AM1 are about 40% less than those given by MNDO.
  - AM1 phosphorus has a spurious and very sharp potential barrier at 3.0Å. The effect of this is to distort otherwise symmetric geometries and to introduce spurious activation barriers. A vivid example is given by P_4O_6, in which the nominally equivalent P-P bonds are predicted by AM1 to differ by 0.4Å. This is by far the most severe limitation of AM1.
  - Alkyl groups have a systematic error due to the heat of formation of the CH_2 fragment being too negative by about 2 kcal/mol.
  - Nitro compounds, although considerably improved, are still systematically too positive in energy.
  - The peroxide bond is still systematically too short by about 0.17Å.

PM3 Applicability and Limitations

PM3 (Parameterized Model revision 3) may be applied to the elements shaded in the following table:



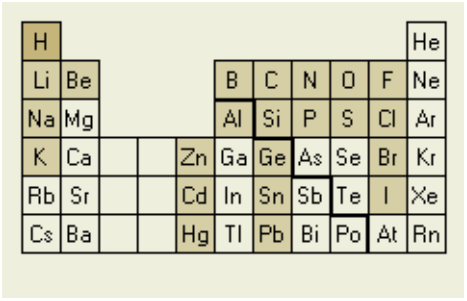
The following apply to PM3:

- PM3 is a reparameterization of AM1.
- PM3 is a distinct improvement over AM1.
- Hypervalent compounds are predicted with considerably improved accuracy.

- Overall errors in ΔH_f are reduced by about 40% relative to AM1.
- Little information exists regarding the limitations of PM3. This should be corrected naturally as results of PM3 calculations are reported.
- The barrier to rotation in formamide is practically non-existent. In part, this can be corrected by the use of the MMOK option. The MMOK option is used by default in CS MOPAC. For more information about MMOK see the online MOPAC Manual.

MNDO-d Applicability and Limitations

MNDO-d (Modified Neglect of Differential Overlap with d-Orbitals) may be applied to the elements shaded in the table below:



MNDO-d is a reformulation of MNDO with an extended basis set to include d-orbitals. This method may be applied to the elements shaded in the table below. Results obtained from MNDO-d are generally superior to those obtained from MNDO. The MNDO method should be used where it is necessary to compare or repeat calculations previously performed using MNDO.

The following types of calculations, as indicated by MOPAC keywords, are incompatible with MNDO-d:

- COSMO (Conductor-like Screening Model) solvation
- POLAR (polarizability calculation)
- GREENF (Green's Function)
- TOM (Miertus-Scirocco-Tomasi self-consistent reaction field model for solvation)

Using Keywords

Selecting parameters for a MOPAC approximation automatically inserts keywords in a window on the **General** tab of the MOPAC Interface. You can edit these keywords or use additional keywords to perform other calculations or save information to the *.out file.

CAUTION

Use the automatic keywords unless you are an advanced MOPAC user. Changing the keywords may give unreliable results.

For a complete list of keywords see the MOPAC online manual.

Automatic Keywords

The following contains keywords automatically sent to MOPAC and some additional keywords you can use to affect convergence.

Keyword	Description
EF	Automatically sent to MOPAC to specify the use of the Eigenvector Following (EF) minimizer.
BFGS	Prevents the automatic insertion of EF and restores the BFGS minimizer.
GEO-OK	Automatically sent to MOPAC to override checking of the Z-matrix.

Keyword	Description
MMOK	Automatically sent to MOPAC to specify Molecular Mechanics correction for amide bonds. Use the additional keyword NOMM to turn this keyword off.
RMAX=n.nn	The calculated/predicted energy change must be less than n.nn. The default is 4.0.
RMIN=n.nn	The calculated/predicted energy change must be more than n.n. The default value is 0.000.
PRECISE	Runs the SCF calculations using a higher precision so that values do not fluctuate from run to run.
LET	Overrides safety checks to make the job run faster.
RECALC=5	Use this keyword if the optimization has trouble converging to a transition state.

For descriptions of error messages reported by MOPAC see Chapter 11, pages 325–331, in the MOPAC manual.

Additional Keywords

Keywords that output the details of a particular computation are shown in the following table. Terms marked with an asterisk (*) appear in the *.out file.

Keyword	Data
ENPART	All Energy Components*
FORCE	Zero Point Energy
FORCE	Vibrational Frequencies*
MECI	Microstates used in MECI calculation*
none	HOMO/LUMO Energies*
none	Ionization Potential*
none	Symmetry*
LOCALIZE	Print localized orbitals
VECTORS	Print final eigenvectors (molecular orbital coefficients)
BONDS	Bond Order Matrix*

The following table contains the keywords that invoke additional computations. Terms marked with an asterisk (*) appear in the *.out file.

Keyword	Description
CIS	UV absorption energies* *NOTE: Performs C.I. using only the first excited Singlet states and does not include the ground state. Use* **MECI** *to print out energy information in the *.out file.*
FORCE	Vibrational Analysis* *NOTE: Useful for determining zero point energies and normal vibrational modes. Use* **DFORCE** *to print out vibration information in *.out file.*
NOMM	No MM correction *NOTE: By default, MOPAC performs a molecular mechanics (MM) correction for CONH bonds.*
PI	Resolve density matrix* *NOTE: Resolve density matrix into sigma and pi bonds.*
PRECISE	Increase SCF criteria *NOTE: Increases criteria by 100 times. This is useful for increasing the precision of energies reported.*
T = n [M,H,D]	Increase the total CPU time allowed for the job. *NOTE: The default is 1h (1 hour) or 3600 seconds.*

Specifying the Electronic Configuration

MOPAC must have the net charge of the molecule in order to determine whether the molecule is open or closed shell. If a molecule has a net charge, be sure you have either specified a charged atom type or added the charge.

CS MOPAC 2002 supports "sparkles"– pure ionic charges that can be used as counter-ions or to form dipoles that mimic solvation effects.

You can assign a charge using the Text Building tool or by specifying it in MOPAC:

To add the charge to the model:

1. Click the Text Building tool.
2. Click an atom in your model.
3. Type a charge symbol.

   For example, click a carbon and type "+" in a text box to make it a carbocation.The charge is automatically sent to MOPAC when you do a calculation.

To specify the charge in MOPAC:

1. From the **Calculations** menu, point to **MOPAC Interface** and choose a computation.

   The MOPAC Interface dialog box appears.

2. On the **General** tab, in the **Keywords** box, type the keyword CHARGE=n, where n is a positive or negative integer (-2, -1, +1, +2).

Different combinations of spin-up (alpha electrons) and spin-down (beta electrons) lead to various electronic energies. These combinations are specified as the Spin Multiplicity of the molecule. The following table shows the relation between total spin S, spin multiplicity, and the number of unpaired electrons.

Spin	Keyword	(# unpaired electrons)
0	SINGLET	0 unpaired
1/2	DOUBLET	1 unpaired
1	TRIPLET	2 unpaired
1 1/2	QUARTET	3 unpaired
2	QUINTET	4 unpaired
2 1/2	SEXTET	5 unpaired

To determine the appropriate spin multiplicity, consider whether:

- The molecule has an even or an odd number of electrons.
- The molecule is in its ground state or an excited state.
- To use RHF or UHF methods.

The following table shows some common permutations of these three factors:

RHF (Closed Shell)

Electronic State	Spin State	Keywords to Use OPEN(n1,n2)[a] ROOT = n C.I.= n	
Ground	SINGLET		
	DOUBLET	1,2	
	TRIPLET	2,2	
	QUARTET	3,3	
	QUINTET	4,4	
	SEXTET	5,5	
1st Excited	SINGLET	2	
	DOUBLET	2	2
	TRIPLET	2	3
	QUARTET	2	4
	QUINTET	2	5
	SEXTET	2	6
2nd Excited	SINGLET	3	
	DOUBLET	3	3
	TRIPLET	3	3
	QUARTET	3	4
	QUINTET	3	5
	SEXTET	3	6

a. The OPEN keyword is necessary only when the molecule has high symmetry, such as molecular oxygen.

UHF (Open Shell)

Electronic State	Spin State
Ground	SINGLET
	DOUBLET

TRIPLET

QUARTET

QUINTET

SEXTET

Even-Electron Systems

If a molecule has an even number of electrons, the ground state and excited state configurations can be Singlet, Triplet, or Quintet (not likely). Normally the ground state is Singlet, but for some molecules, symmetry considerations indicate a Triplet is the most stable ground state.

Ground State, RHF

The Ground State, RHF configuration is as follows:

- Singlet ground state—the most common configuration for a neutral, even electron stable organic compound. No additional keywords are necessary.
- Triplet ground state—Use the following keyword combination: TRIPLET OPEN(2,2)
- Quintet ground state—Use the following keyword combination: QUINTET OPEN(4,4)

NOTE: *The OPEN keyword is normally necessary only when the molecule has a high degree of symmetry, such as molecular oxygen. The OPEN keyword increases the active space available to the SCF calculation by including virtual orbitals. This is necessary for attaining the higher multiplicity configurations for even shell system. The OPEN keyword also invokes the RHF computation using the 1/2 electron approximation method and a C.I. calculation to correct the final RHF energies. To see the states used in a C.I. calculation, type MECI as an additional keyword. The information is printed at the bottom of the *.out file.*

Ground State, UHF

For UHF computations, all unpaired electrons are forced to be spin up (alpha).

- Singlet ground state—the most common configuration for a neutral, even electron, stable organic compound. No additional keywords are necessary.
- UHF will likely converge to the RHF solution for Singlet ground states.
- Triplet or Quintet ground state: Use the keyword TRIPLET or QUINTET.

NOTE: *When a higher multiplicity is used, the UHF solution yields different energies due to separate treatment of alpha electrons.*

Excited State, RHF

First Excited State: The first excited state is actually the second lowest state (the root=2) for a given spin system (Singlet, Triplet, Quintet).

To request the first excited state, use the following sets of keywords:

First excited Singlet: ROOT=2 OPEN(2,2) SINGLET (or specify the single keyword EXCITED)

First excited triplet: ROOT=2 OPEN (2,2) TRIPLET C.I.=n, where n=3 is the simplest case.

First excited quintet: ROOT=2 OPEN (4,4) QUINTET C.I.=n, where n=5 is the simplest case.

Second Excited State: The second excited state is actually the third lowest state (the root=3) for a given system (Singlet, Triplet, Quintet). To request the second excited state use the following set of keywords:

Second excited Singlet: OPEN(2,2) ROOT=3 SINGLET

Second excited triplet: OPEN(2,2) ROOT=3 TRIPLET C.I.=n, where n=3 is the simplest case.

Second excited quintet: OPEN(4,4) ROOT=3 QUINTET C.I.=n, where n=5 is the simplest case.

Excited State, UHF

Only the ground state of a given multiplicity can be calculated using UHF.

Odd-Electron Systems

Often, anions, cations, or radicals are odd-electron systems. Normally, the ground states and excited state configuration can be doublet, quartet or sextet.

Ground State, RHF

Doublet ground state: This is the most common configuration. No additional keywords are necessary.

Quartet: Use the following keyword combination: QUARTET OPEN(3,3)

Sextet ground state: Use the following keyword combination: SEXTET OPEN(5,5)

Ground State, UHF

For UHF computations all unpaired electrons are forced to be spin up (alpha).

Doublet ground state: This is the most common configuration for a odd electron molecule. No additional keywords are necessary.

UHF will yield energies different from those obtained by the RHF method.

Quartet and Sextet ground state: Use the keyword QUARTET or SEXTET.

Excited State, RHF

First Excited State: The first excited state is actually the second lowest state (the root=2) for a given spin system (Doublet, Quartet, Sextet). To request the first excited state use the following sets of keywords.

First excited doublet: ROOT=2 DOUBLET C.I.=n, where n=2 is the simplest case.

First excited quartet: ROOT=2 QUARTET C.I.=n, where n=4 is the simplest case.

First excited sextet: ROOT=2 SEXTET C.I.=n, where n=5 is the simplest case.

Second Excited State: The second excited state is actually the third lowest state (the root=3) for a given system (Singlet, Triplet, Quintet). To request the second excited state use the following set of keywords:

Second excited doublet: ROOT=3 DOUBLET C.I.=n, where n=3 is the simplest case.

Second excited quartet: ROOT=3 QUARTET C.I.=n, where n=4 is the simplest case.

Second excited sextet: ROOT=3 SEXTET C.I.=n, where n=5 is the simplest case.

NOTE: *If you get an error indicating the active space is not spanned, use C.I.> n for the simplest case to increase the number of orbitals available in the active space. To see the states used in a C.I. calculation, type MECI as an additional keyword. The information is printed at the bottom of the *.out file.*

Excited State, UHF

Only the ground state of a given multiplicity can be calculated using UHF.

Sparkles

Sparkles are used to represent pure ionic charges. They are roughly equivalent to the following chemical entities:

Chemical symbol	Equivalent to...
+	tetramethyl ammonium, potassium or cesium cation + electron

Chemical symbol	Equivalent to...
++	barium di-cation + 2 electrons
_	borohydride halogen, or nitrate anion minus electron
=	sulfate, oxalate di-anion minus 2 electrons

Sparkles are represented in Chem3D by adding a charged dummy atom to the model.

TIP: *Dummy atoms are created with the uncoordinated bond tool. You must add the charge after creating the dummy.*

The output file shows the the chemical symbol as XX.

ATOM NUMBER	CHEMICAL SYMBOL	X (ANGSTROMS)
1	C	1.23440000
2	C	0.00660000
3	C	0.30460000
4	C	-0.77340000
5	O	-0.52830000
6	O	-1.88750000
7	XX	2.19333900
8	O	1.08280000
9	N	-1.14510000

Optimizing Geometry

Chem3D uses the Eigenvector Following (EF) routine as the default geometry optimization routine for minimization calculations. EF is generally superior to the other minimizers, and is the default used by MOPAC 2002. (Earlier versions of MOPAC used BFGS as the default.) The other alternatives are described below.

TS

The TS optimizer is used to optimize a transition state. It is inserted automatically when you select **Optimize to Transition State** from the **MOPAC Interface** submenu.

BFGS

For large models (over about 500-1,000 atoms) the suggested optimizer is the Broyden-Fletcher-Goldfarb-Shanno procedure. By specifying BFGS, this procedure will be used instead of EF.

LBFGS

For very large systems, the LBFGS optimizer is often the only method that can be used. It is based on the BFGS optimizer, but calculates the inverse Hessian as needed rather than storing it. Because it uses little memory, it is preferred for optimizing very large systems. It is, however, not as efficient as the other optimizers.

MOPAC Files

CS MOPAC can use standard MOPAC text files for input, and creates standard MOPAC output files. These are especially useful when running repeat computations.

Using the *.out file

In addition to the Messages window, MOPAC creates two text files that contain information about the computations.

Each computation performed using MOPAC creates a *.out file containing all information concerning the computation. A summary *.arax file is also created, (where x increments from a to z after each run). The *.out file is overwritten for each run, but a new summary *.arax, file is created after each computation (*.araa, *.arab, and so on.)

The .out and .aax files are saved by default to the **\Mopac Interface** subfolder in your **My Documents** folder. You may specify a different location from the **General** tab of the Mopac Interface dialog box.The following information is found in the summary file for each run:

- Electronic Energy ($E_{electronic}$)
- Core-Core Repulsion Energy ($E_{nuclear}$)
- Symmetry
- Ionization Potential
- HOMO/LUMO energies

The *.out file contains the following information by default.

- Starting atomic coordinates
- Starting Z-matrix
- Molecular orbital energies (eigenvalues)
- Ending atomic coordinates

The workings of many of the calculations can also be printed in the *.out file by specifying the appropriate keywords before running the calculation. For example, specifying MECI as an additional keyword will show the derivation of microstates used in an RHF 1/2 electron approximation calculation. For more information see "Using Keywords" on page 170.

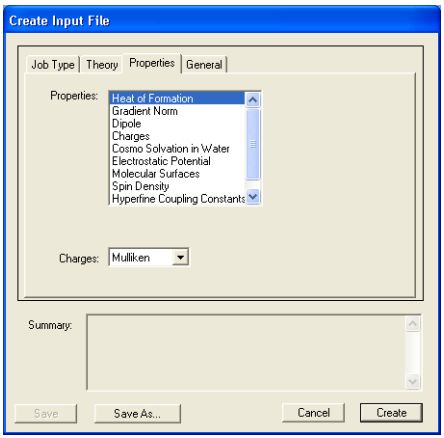
NOTE: *Close the *.out file while performing MOPAC computations or the MOPAC application stops functioning.*

Creating an Input File

A MOPAC input file (.MOP) is associated with a model and its dialog box settings.

To create a MOPAC input file:

1. From the **MOPAC Interface** submenu of the **Calculations** menu, choose **Create Input File**.



2. Select the appropriate settings and click **Create**.

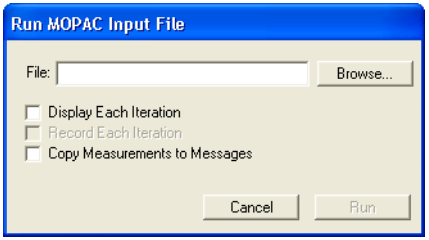
Running Input Files

Chem3D allows you to run previously created MOPAC input files.

To run an input file:

1. From the **MOPAC Interface** submenu of the **Calculations** menu, click **Run Input File**.

   The **Run MOPAC Input File** dialog box appears.



2. Type the full path of the MOPAC file or Browse to the file location.
3. Select the appropriate options. For more information about the options see "Specifying the Electronic Configuration" on page 172.

4. Click **Run**.

   A new model window appears displaying the initial model. The MOPAC job runs and the results appear.

   All properties requested for the job appear in the *.out file. Only iteration messages appear for these jobs.

NOTE: *If you are opening a MOPAC file where a model has an open valence, such as a radical, you can avoid having the coordinates readjusted by Chem3D by turning off Automatically Rectify in the Building control panel.*

NOTE: *MOPAC input files that containing multiple instances of the Z-matrix under examination will not be correctly displayed in Chem3D. This type of MOPAC input files includes calculations that use the SADDLE keyword, or model reaction coordinate geometries.*

Running MOPAC Jobs

Chem3D enables you to select a previously created MOPAC job description file (.jdf). The .jdf file can be thought of as a set of Settings that apply to a particular dialog box. For more information about .jdf files see "JDF Files" on page 126.

To create a .jdf file:

1. From the **MOPAC Interface** submenu of the Calculations menu, choose a calculation.
2. After all settings for the calculation are specified, click **Save As**.

To run a MOPAC job from a .jdf file:

1. From the **MOPAC Interface** submenu of the Calculations menu, click **Run MOPAC Job**.

   The Open dialog box appears.
2. Select the .jdf file to run.

   The dialog box corresponding to the type of job saved within the file appears.
3. Click **Run**.

Repeating MOPAC Jobs

After you perform a MOPAC calculation, you can repeat the job as follows:

4. From the **MOPAC Interface** submenu of the Calculations menu, choose **Repeat** [*name of computation*].

   The appropriate dialog box appears.
5. Change parameters if desired and click **Run**.

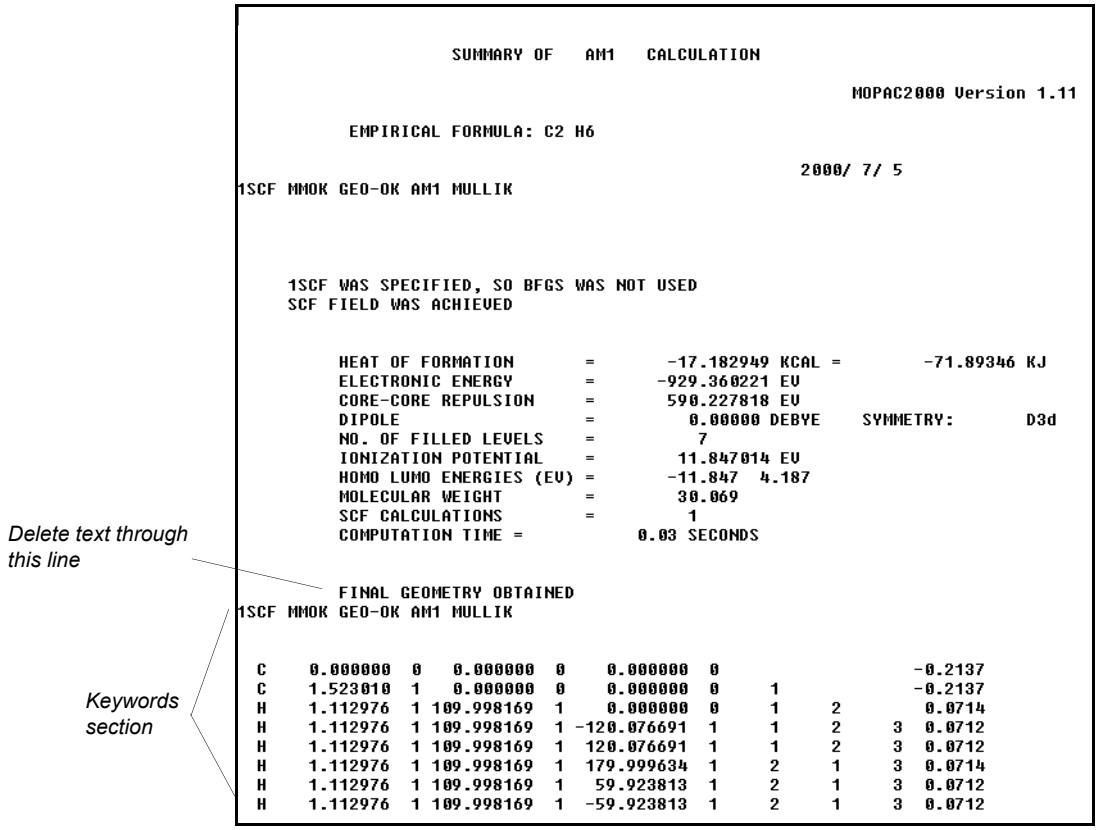
   The computation proceeds.

Creating Structures From .arc Files

When you perform a MOPAC calculation, the results are stored in an .arc file in the **\Mopac Interface** subfolder in your **My Documents** folder.

You can create a structure from the .arc file as follows:

1. Open the .arc file in a text editor.
2. Delete the text above the keywords section of the file as shown in the following illustration.
3. Save the file with a .mop extension.
4. Open the .mop file.

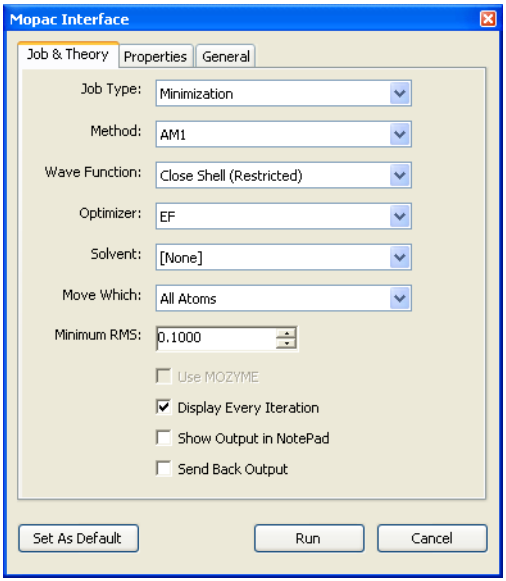

SUMMARY OF AM1 CALCULATION
MOPAC2000 Version 1.11
EMPIRICAL FORMULA: C2 H6
2000/ 7/ 5
1SCF MMOK GEO-OK AM1 MULLIK
1SCF WAS SPECIFIED, SO BFGS WAS NOT USED
SCF FIELD WAS ACHIEVED
HEAT OF FORMATION = -17.182949 KCAL = -71.89346 KJ
ELECTRONIC ENERGY = -929.360221 EV
CORE-CORE REPULSION = 590.227818 EV
DIPOLE = 0.00000 DEBYE SYMMETRY: D3d
NO. OF FILLED LEVELS = 7
IONIZATION POTENTIAL = 11.847014 EV
HOMO LUMO ENERGIES (EV) = -11.847 4.187
MOLECULAR WEIGHT = 30.069
SCF CALCULATIONS = 1
COMPUTATION TIME = 0.03 SECONDS
FINAL GEOMETRY OBTAINED
1SCF MMOK GEO-OK AM1 MULLIK
C 0.000000 0 0.000000 0 0.000000 0 -0.2137
C 1.523010 1 0.000000 0 0.000000 0 1 -0.2137
H 1.112976 1 109.998169 1 0.000000 0 1 2 0.0714
H 1.112976 1 109.998169 1 -120.076691 1 1 2 3 0.0712
H 1.112976 1 109.998169 1 120.076691 1 1 2 3 0.0712
H 1.112976 1 109.998169 1 179.999634 1 2 1 3 0.0714
H 1.112976 1 109.998169 1 59.923813 1 2 1 3 0.0712
H 1.112976 1 109.998169 1 -59.923813 1 2 1 3 0.0712
Delete text through this line
Keywords section

Minimizing Energy

Minimizing energy is generally the first molecular computation performed on a model.

From the **Calculations** menu, point to **MOPAC Interface** and choose **Minimize Energy**.

The MOPAC Interface dialog box appears, with **Minimize** as the default **Job Type**.



You may use the defaults, or set your own parameters.

Option	Function
Job Type	Sets defaults for different types of computations.
Method	Selects a method. See "Choosing a Hamiltonian" on page 167 for descriptions of the methods.
Wave Function	Selects close or open shell. See "Specifying the Electronic Configuration" on page 172 for more details.
Optimizer	Selects a geometry minimizer. See "Optimizing Geometry" on page 176 for more information.
Solvent	Selects a solvent. For more information on solvent effects, see the online MOPAC manual.
Move Which	Allows you to minimize part of a model by selecting it.
Minimum RMS	Specifies the convergence criteria for the gradient of the potential energy surface. (See also "Gradient Norm" on page 185.)
Use MOZYME	ULTRA For very large models, alters the way the SCF is generated, cutting memory requirements and running much faster.

Option	Function
Display Every Iteration	Displays the minimization process "live" at each iteration in the calculation. NOTE: Adds significantly to the time required to minimize the structure.
Show Output in Notepad	Sends the output to a text file.
Send Back Output	Displays the value of each measurement in the Output window. NOTE: Adds significantly to the time required to minimize the structure.

Notes

RMS—The default value of 0.100 is a reasonable compromise between accuracy and speed. Reducing the value means that the calculation continues longer as it tries to get even closer to a minimum. Increasing the value shortens the calculation, but leaves you farther from a minimum. Increase the value if you want a better optimization of a conformation that you know is not a minimum, but you want to isolate it for computing comparative data.

NOTE: *If you want to use a value <0.01, you must specify LET in the keywords section (General Tab).*

Wave Function—Selecting a wave function from the drop down menu involves deciding whether to use RHF or UHF computations.

RHF is the default Hartree-Fock method used for closed shell systems. To use RHF select the **Close Shell (Restricted)** wave function.

UHF is an alternative form of the HF method used for open shell systems. To use UHF select the **Open Shell (Unrestricted)** wave function. If you wish to calculate Hyperfine Coupling Constants, you must select the UHF wave function.

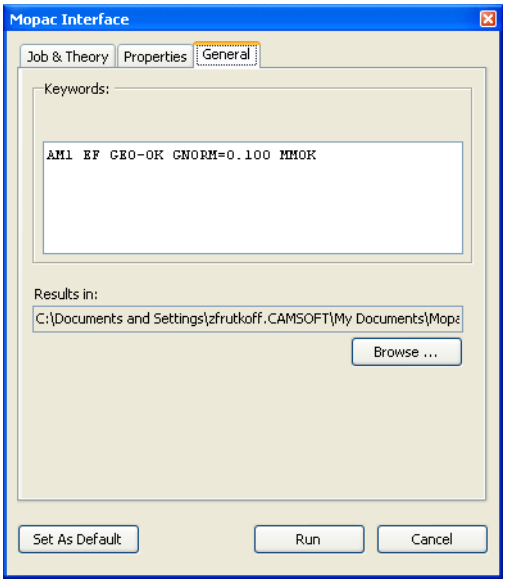
NOTE: *UHF computations take at least twice as long as RHF. This may be the deciding consideration of method when large molecules are being studied.*

Adding Keywords

Click the **General** tab to specify additional MOPAC keywords. This will tailor a calculation to more exacting requirements. For example, you might use additional keywords to control convergence

criteria, to optimize to an excited state instead of the ground state, or to calculate additional properties.

NOTE: *Other properties that you might specify through the keywords section of the dialog box may affect the outcome. For more information see "Using Keywords" on page 170.*



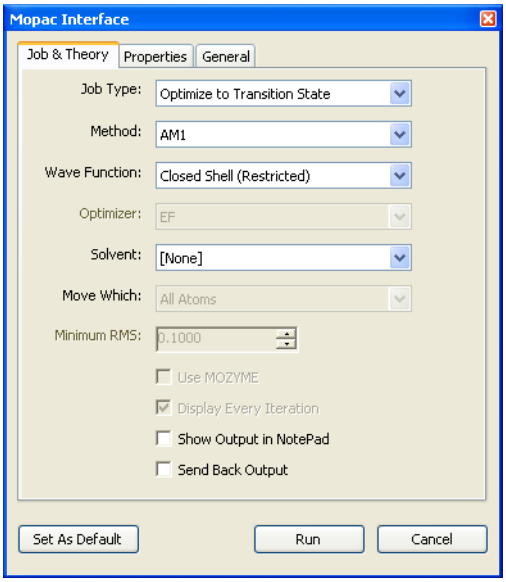
Optimize to Transition State

To optimize your model to a transition state, use a conformation that is as close to the transition state as possible. Do not use a local or global minimum, because the algorithm cannot effectively move the geometry from that starting point.

To optimize a transition state:

1. Choose **Optimize to Transition State** from the **MOPAC Interface** submenu of the **Calculations** menu.

   The MOPAC Interface dialog box appears.



2. On the **Job and Theory** tab select a **Method** and **Wave Function**.

   NOTE: *Unless you are an experienced MOPAC user, use the Transition State defaults.*

3. On the **Properties** tab, select the properties you wish to calculate from the final optimized conformation.
4. On the **General** tab, type any additional keywords that you want to use to modify the optimization.
5. Click **Run**.

   The information about the model and the keywords are sent to MOPAC. If you have selected **Send Back Output**, the Output window appears.

The Output window displays intermediate messages about the status of the minimization. A message appears if the minimization terminates abnormally, usually due to a poor starting conformation.

The following contains keywords automatically sent to MOPAC and some additional keywords you can use to affect convergence.

Keyword	Description
EF	Automatically sent to MOPAC to specify the use of the Eigenvector Following minimizer.
GEO-OK	Automatically sent to MOPAC to override checking of the Z-matrix.
MMOK	Automatically sent to MOPAC to specify Molecular Mechanics correction for amide bonds. Use the additional keyword NOMM to turn this keyword off.
RMAX=n.nn	The calculated/predicted energy change must be less than n.nn. The default is 4.0.
RMIN=n.nn	the calculated/predicted energy change must be more than n.n. The default value is 0.000.
PRECISE	Runs the SCF calculations using a higher precision so that values do not fluctuate from run to run.
LET	Overrides safety checks to make the job run faster (or further).
RECALC=5	Use this keyword if the optimization has trouble converging to a transition state.

For descriptions of error messages reported by MOPAC see Chapter 11, pages 325–331, in the MOPAC manual.

To interrupt a minimization that is in progress:

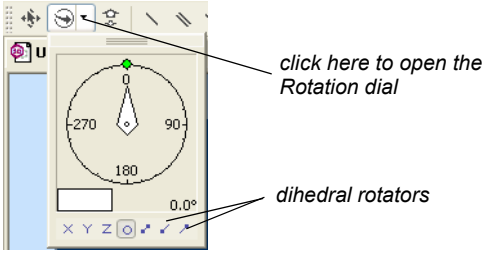
- Click **Stop** in the Movie Controller.

Example:

Locating the Eclipsed Transition State of Ethane

Build a model of ethane:

1. From the File menu, choose **New Model**
2. Double-click in the model window.
   A text box appears.
3. Type CH3CH3 and press the **Enter** key.
   A model of ethane appears.
4. Select the Rotation tool.
5. Click the arrow next to the Rotation tool, and drag down the Rotation dial.



6. Hold down the S key and select the bond between the C(1) and C(2) atoms.

   NOTE: *Holding down the S key temporarily activates the Select tool.*

7. Select one of the dihedral rotators, then enter 57 in the text box and press the Enter key.

   A nearly eclipsed conformation of ethane is displayed.

   TIP: *To view this better, rotate the model on the Y axis until the carbon atoms are aligned.*

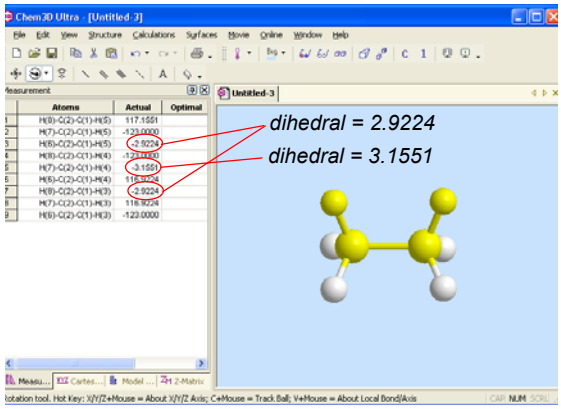
Use Mopac to create the precise eclipsed transition state:

8. Holding down the S and shift keys, click on any two nearly eclipsed hydrogen atoms, such as H(4) and H(7), to identify the dihedral to track.

   You should have a nearly coplanar four-atom chain, such as H(4)-C(1)-C(2)-H(7), selected.

9. From the **Structure** menu, point to **Measurements**, and choose **Dihedral Angle**.

   The Measurements table appears and displays an actual value for the selected dihedral angle of about 3 degrees (this will vary slightly between experiments).



10. From the **MOPAC Interface** submenu of the **Calculations** menu, choose **Optimize to Transition State**.

11. Click the **Copy Measurements to Messages** box on the **Job Type** tab.

12. Click **Run**.

    The ethane model minimizes so that the dihedral is 0 degrees, corresponding to the eclipsed conformation of ethane, a known transition state between the staggered minima conformations.

To see the Newman projection of the eclipsed ethane model:

1. Select both carbon atoms.
2. From **View Position** submenu of the **View** menu, click **Align View Z-Axis With Selection**.

   NOTE: *If you perform an Energy Minimization from the same starting dihedral, your model would optimize to the staggered conformation of ethane where the dihedral is 60 degrees, instead of optimizing to the transition state.*

Computing Properties

To perform a single point calculation on the current conformation of a model:

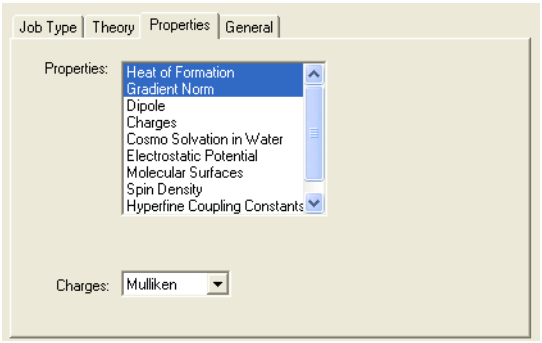
1. From the **MOPAC Interface** submenu of the **Calculations** menu, choose **Compute Properties**.

   The Compute Properties dialog box appears.

2. On the **Theory** tab, choose a potential energy function to use for performing the calculation.

NOTE: *For more information about the potential energy functions available in MOPAC see "Computation Concepts"*

3. On the **Properties** tab, select the properties to calculate.



4. On the **Properties** tab, set the **charges**.
5. On the **General** tab, type any additional keywords, if necessary.
6. Click **Run**.

MOPAC Properties

The following section describes the properties that you can calculate for a given conformation of your model, either as a single point energy computation using the Compute Properties command, or after a minimization using either the Minimize Energy or Optimize to Transition State commands.

Heat of Formation, ΔH_f

This energy value represents the heat of formation for a model's current conformation. It is useful for comparing the stability of conformations of the same model.

NOTE: *The heat of formation values include the zero point energies. To obtain the zero point energy for a conformation run a force operation using the keyword FORCE. The zero-point energy is found at the bottom of the *.out file.*

The heat of formation in MOPAC is the gas-phase heat of formation at 298K of one mole of a compound from its elements in their standard state.

The heat of formation is composed of the following terms:

$$\Delta H_f = E_{elec} + E_{nucl} - E_{isol} - E_{atoms}$$

Where:

- E_{elec} is calculated from the SCF calculation.
- E_{nucl} is the core-core repulsion based on the nuclei in the molecule.
- E_{isol} and E_{atoms} are parameters supplied by the potential function for the elements within your molecule.

NOTE: *You can use the keyword ENPART and open the *.out file at the end of a run to view the energy components making up the heat of formation and SCF calculations. See the MOPAC online manual reference page 137, for more information.*

Gradient Norm

This is the value of the scalar of the vector of derivatives with respect to the geometric variables flagged for optimization. This property (called GNORM in the MOPAC manual) is automatically selected for a minimization, which calculates the GNORM and compares it to the selected minimum gradient. When the selected minimum is reached, the minimization terminates.

Selecting this property for a Compute Properties operation (where a minimization is not being performed) will give you an idea of how close to optimum geometry the model is for the particular calculation.

NOTE: *The GNORM property is not the same as the MOPAC keyword GNORM. For more information see the MOPAC manual, pages 31 and 180.*

Dipole Moment

The dipole moment is the first derivative of the energy with respect to an applied electric field. It measures the asymmetry in the molecular charge distribution and is reported as a vector in three dimensions.

The dipole value will differ when you choose Mulliken Charges, Wang-Ford Charges or Electrostatic Potential, as a different density matrix is used in each computation.

NOTE: *For more information see the MOPAC manual, page 119.*

The following table contains the keywords automatically sent to MOPAC.

Keyword	Description
GEO-OK	Automatically sent to MOPAC to override checking of the Z-matrix.
MMOK	Automatically sent to MOPAC to specify Molecular Mechanics correction for amide bonds. Use the additional keyword NOMM to turn this keyword off.

Charges

The property, Charges, determines the atomic charges using a variety of techniques discussed in the following sections. In this example the charges are the electrostatic potential derived charges from Wang-Ford, because Wang-Ford charges give useful information about chemical stability (reactivity).

Mulliken Charges

This property provides a set of charges on an atom basis derived by reworking the density matrix from the SCF calculation. Unlike the Wang-Ford charges utilized in the previous example, Mulliken charges give a quick survey of charge distribution in a molecule.

NOTE: *For more information, see the MOPAC online manual, page 41 and 121.*

The following table contains the keywords automatically sent to MOPAC.

Keyword	Description
MULLIK	Automatically sent to MOPAC to generate the Mulliken Population Analysis.
GEO-OK	Automatically sent to MOPAC to override checking of the Z-matrix.
MMOK	Automatically sent to MOPAC to specify Molecular Mechanics correction for amide bonds. Use the additional keyword NOMM to turn this keyword off.

Charges From an Electrostatic Potential

The charges derived from an electrostatic potential computation give useful information about chemical reactivity.

The electrostatic potential is computed by creating an electrostatic potential grid. Chem3D reports the point charges derived from such a grid.

In general, these atomic point charges give a better indication of likely sites of attack when compared to atomic charges derived from the Coulson density

matrix (Charges) or Mulliken population analysis (Mulliken Charges). The uses for electrostatic potential derived charges are generally the same as for atomic charges. For examples, see "Charges" on page 186.

There are two properties available for calculating atomic point charges: Wang-Ford Charges and Electrostatic Potential.

Wang-Ford Charges

This computation of point charges can be used with the AM1 potential function only.

For information about the elements covered using the AM1 potential function see "" and the MOPAC online manual, page 223.

NOTE: *For elements not covered by the AM1 potential function, use the Electrostatic Potential property to get similar information on elements outside this properties range.*

Below are the keywords automatically sent to MOPAC.

Keyword	Description
PMEP	Automatically sent to MOPAC to specify the generation of Point Charges from PMEP.
QPMEP	Automatically sent to MOPAC to specify the Wang/Ford electrostatic Potential routine.
GEO-OK	Automatically sent to MOPAC to override checking of the Z-matrix.
MMOK	Automatically sent to MOPAC to specify Molecular Mechanics correction for amide bonds. Use the additional keyword NOMM to turn this keyword off.

Electrostatic Potential

Use the electrostatic potential property when the element coverage of the AM1 potential function does not apply to the molecule of interest. For more information see the MOPAC online manual, page 223.

The following table contains the keywords automatically sent to MOPAC and those you can use to affect this property.

Keyword	Description
ESP	Automatically sent to MOPAC to specify the Electrostatic Potential routine.
POTWRT	Add this keyword if you want to print out the ESP map values.
GEO-OK	Automatically sent to MOPAC to override checking of the Z-matrix.
MMOK	Automatically sent to MOPAC to specify Molecular Mechanics correction for amide bonds. Use the additional keyword NOMM to turn this keyword off.

Molecular Surfaces

Molecular surfaces calculate the data necessary to render the Total Charge Density, Molecular Electrostatic Potential, Spin Density, and Molecular Orbitals surfaces.

Polarizability

The polarizability (and hyperpolarizability) property provides information about the distribution of electrons based on presence of an applied electric field. In general, molecules with more delocalized electrons have higher values for this property.

Polarizability data is often used in other equations for evaluation of optical properties of molecules. For more information see the MOPAC online manual, page 214.

The polarizability and hyperpolarizability values reported are the first order (alpha) tensors (xx, yy, zz, xz, yz, xy), second order (beta) tensors and third order (gamma) tensors.

NOTE: *Polarizabilities cannot be calculated using the MINDO/3 potential function.*

COSMO Solvation in Water

The COSMO method is useful for determining the stability of various species in a solvent. The default solvent is water. For more information, see the MOPAC online manual.

To run the COSMO method, make the following selections in the MOPAC Interface:

- On the Job & Theory tab, select COSMO in the **Solvent** field.
- On the Properties tab, check the **COSMO Area** and/or **COSMO Volume** properties. You must check each property you want to see in the results.

NOTE: *You can also use the Miertus-Scirocco-Tomasi solvation model, which is available using the H2O keyword. This method is recommended only for water as the solvent. A discussion of this method can be found in the MOPAC online documentation.*

Hyperfine Coupling Constants

Hyperfine Coupling Constants are useful for simulating Electron Spin Resonance (ESR) spectra.

Hyperfine interaction of the unpaired electron with the central proton and other equivalent protons cause complex splitting patterns in ESR spectra. ESR spectroscopy measures the absorption of microwave radiation by an unpaired electron when it is placed under a strong magnetic field.

Hyperfine Coupling Constants (HFCs) are related to the line spacing within the hyperfine pattern of an ESR spectra and the distance between peaks.

Species that contain unpaired electrons are as follows:

- Free radicals
- Odd electron molecules
- Transition metal complexes
- Rare-earth ions
- Triplet-state molecules

For more information see the MOPAC online manual, page 34.

The following table contains the keywords automatically sent to MOPAC and those you can use to affect this property.

Keyword	Description
UHF	Automatically sent to MOPAC if you choose "Open Shell (Unrestricted)" wave functions to specify the use of the Unrestricted Hartree-Fock methods.
Hyperfine	Automatically sent to MOPAC to specify the hyperfine computation.
GEO-OK	Automatically sent to MOPAC to override checking of the Z-matrix.
MMOK	Automatically sent to MOPAC to specify Molecular Mechanics correction for amide bonds. Use the additional keyword NOMM to turn this keyword off.

Spin Density

Spin density arises in molecules where there is an unpaired electron. Spin density data provides relative amounts of alpha spin electrons for a particular state.

Spin density is a useful property for accessing sites of reactivity and for simulating ESR spectra.

Two methods of calculating spin density of molecules with unpaired electrons are available: RHF Spin Density and UHF Spin Density.

UHF Spin Density

The UHF Spin Density removes the closed shell restriction. In doing so, separate wave functions for alpha and beta spin electrons are computed. For more information see the MOPAC online manual, page 152.

The following table contains the keywords automatically sent to MOPAC and those you can use to affect this property.

Keyword	Description
UHF	Automatically sent to MOPAC if you choose "Open Shell (Unrestricted)" wave functions to specify the use of the Unrestricted Hartree-Fock methods.
GEO-OK	Automatically sent to MOPAC to override checking of the Z-matrix.
MMOK	Automatically sent to MOPAC to specify Molecular Mechanics correction for amide bonds. Use the additional keyword NOMM to turn this keyword off.
SPIN	You can add this keyword to print the spin density matrix in the *.out file.

RHF Spin Density

RHF Spin Density uses the 1/2 electron correction and a single configuration interaction calculation to isolate the alpha spin density in a molecule. This method is particularly useful when the UHF Spin Density computation becomes too resource intensive for large molecules. For more information see the MOPAC online manual, page 28.

The following table contains the keywords automatically sent to MOPAC and those you can use to affect this property.

Keyword	Description
ESR	Automatically sent to MOPAC to specify RHF spin density calculation.
GEO-OK	Automatically sent to MOPAC to override checking of the Z-matrix.
MMOK	Automatically sent to MOPAC to specify Molecular Mechanics correction for amide bonds. Use the additional keyword NOMM to turn this keyword off.

Example 1

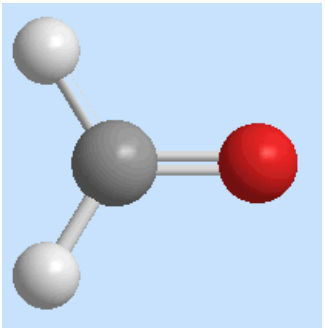
The Dipole Moment of Formaldehyde

To calculate the dipole moment of formaldehyde:

1. From the **File** menu, choose **New Model**.
2. Click the **Text Building** tool.
3. Click in the model window.

   A text box appears.
4. Type H2CO and press the **Enter** key.

   A model of formaldehyde appears.



5. From the **MOPAC Interface** menu of the **Calculations** menu, choose **Minimize Energy**.
6. On the **Theory** tab, choose **AM1**.
7. On the **Properties** tab, select **Dipole**.
8. Click **Run**.

The results shown in the Messages window indicate the electron distribution is skewed in the direction of the oxygen atom.

	X	Y	Z	Total
Dipole (vector Debye)	-2.317	0.000	-0.000	2.317

If you rotate your model, the X,Y, and Z components of the dipole differ. However, the total dipole does not. In this example, the model is oriented so that the significant component of the dipole lies along the X-axis.

Example 2

Comparing Cation Stabilities in a Homologous Series of Molecules

To build the model:

1. From the File menu, choose **New Model**.
2. Click the Text Building tool.
3. Click in the model window.

   A text box appears.
4. For tri-chloro, type CCl3 and press the **Enter** key.
5. Repeat step 1 through step 4 for the other cations: type CHCl2 for di-chloro; type CH2Cl for mono-chloro and CH3 for methyl cation.

   NOTE: *The cations in this example are even electron closed shell systems and are assumed to have Singlet ground state. No modifications through additional keywords are necessary. The default RHF computation is used.*
6. For each model, click the central carbon, type "+" and press the **Enter** key.

   The model changes to a cation and insures that the charge is sent to MOPAC.

To perform the computation:

1. From the **MOPAC Interface** submenu of the Calculations menu, choose **Minimize Energy**.
2. On the Theory tab, choose **AM1**.
3. On the Properties tab, select **Charges** in the Properties list.
4. Select **Wang-Ford** from the Charges list.
5. Click **Run**.

   The results for the model appear in the Message window when the computation is complete.

The molecules are now planar, reflecting sp^2 hybridization of the central carbon.

The following table shows the results:

tri-chloro cation		di-chloro cation		mono-chloro cation		methyl cation	
C(1)	0.03660	C(1)	0.11255	C(1)	0.32463	C(1)	0.72465
Cl(2)	0.31828	Cl(2)	0.33189	Cl(2)	0.35852	H(2)	0.08722
Cl(3)	0.32260	Cl(3)	0.33171	H(3)	0.15844	H(3)	0.09406
Cl(4)	0.32253	H(4)	0.22384	H(4)	0.15841	H(4)	0.09406

From these simple computations, you can reason that the charge of the cation is not localized to the central carbon, but is rather distributed to different extents by the other atoms attached to the charged carbon. The general trend for this group of cations is that the more chlorine atoms attached to the charged carbon, the more stable the cation (the decreasing order of stability is tri-chloro >di-chloro > mono-chloro > methyl).

Example 3

Analyzing Charge Distribution in a Series Of Mono-substituted Phenoxy Ions

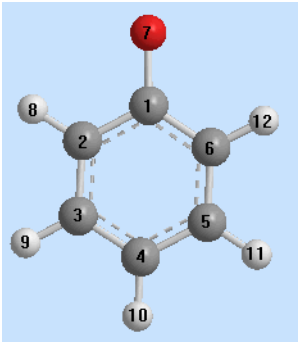
1. From the File menu, choose **New Model**.
2. Click the **Text Building** tool.

3. Click in the model window.

   A text box appears.

4. Type PhO- and press the **Enter** key.

   A phenoxide ion model appears.



NOTE: *All the monosubstituted phenols under examination are even electron closed shell systems and are assumed to have Singlet ground state. No modifications by additional keywords are necessary. The default RHF computation is used.*

5. From the **MOPAC Interface** submenu of the **Calculations** menu, choose **Minimize Energy**.
6. On the Theory tab, choose **PM3**. This automatically selects **Mulliken** from the Charges list.
7. On the Property tab, select **Charges**.
8. Click **Run**.

To build para-nitrophenoxide ion:

1. Click the **Text Building** tool.
2. Click **H10,** type NO2, and then press the **Enter** key.

   Para nitrophenoxide ion is formed.

Perform minimization as in the last step.

- For the last two monosubstituted nitro phenols, first, select the nitro group using the Select Tool and press the Delete key. Add the **nitro group** at the meta (H9) or ortho (H8) position and repeat the analysis.

The data from this series of analyses are shown below. The substitution of a nitro group at para, meta and ortho positions shows a decrease in negative charge at the phenoxy oxygen in the order meta>para>ortho, where ortho substitution shows the greatest reduction of negative charge on the phenoxy oxygen. You can reason from this data that the phenoxy ion is stabilized by nitro substitution at the ortho position.

Phenoxide	p-Nitro	m- Nitro	o-Nitro
C1 0.39572	C1 0.41546	C1 0.38077	C1 0.45789
C2 -0.46113	C2 -0.44929	C2 -0.36594	C2 -0.75764
C3 -0.09388	C3 -0.00519	C3 -0.33658	C3 0.00316
C4 -0.44560	C4 -0.71261	C4 -0.35950	C4 -0.41505
C5 -0.09385	C5 -0.00521	C5 -0.10939	C5 -0.09544
C6 -0.46109	C6 -0.44926	C6 -0.41451	C6 -0.38967
O7 -0.57746	O7 -0.49291	O7 -0.54186	O7 -0.48265
H8 0.16946	H8 0.18718	H8 0.21051	N8 1.38805
H9 0.12069	H9 0.17553	N9 1.31296	H9 0.16911
H10 0.15700	N10 1.38043	H10 0.19979	H10 0.17281
H11 0.12067	H11 0.17561	H11 0.14096	H11 0.13932
H12 0.16946	H12 0.18715	H12 0.17948	H12 0.18090
	O13 -0.70347	O13 -0.65265	O13 -0.71656
	O14 -0.70345	O14 -0.64406	O14 -0.65424

Example 4

Calculating the Dipole Moment of meta-Nitrotoluene

Create a model of *m*-nitrotoluene:

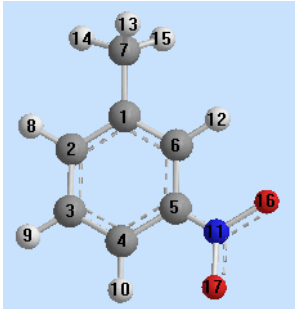
1. From the File menu, choose **New Model**.
2. Click the Text Building tool.
3. Click in the model window.

   A text box appears.
4. Type PhCH3 and press the **Enter** key.

   A model of toluene appears. Reorient the model using the Trackball tool until it is oriented like the model shown in step 8.
5. From the Edit menu, choose **Select All**.
6. Select **Show Serial Numbers** from the Model Display submenu of the View menu.

   NOTE: *Show Serial Numbers is a toggle. When it is selected, the number 1 displays in a frame.*
7. With the Text Building tool, click **H(11)**, and then type NO2 in the text box that appears.
8. Press the **Enter** key.

   A model of *m*-nitrotoluene appears.



Use MOPAC to find the dipole moment:

1. From the **MOPAC Interface** submenu of the Calculations menu, choose **Minimize Energy**.
2. On the Theory tab, choose **AM1**.
3. On the Property tab, select **Polarizabilities**.
4. Click Run.

The following table is a subset of the results showing the effect of an applied electric field on the first order polarizability for *m*-nitrotoluene.

Applied field (eV)	alpha xx	alpha yy	alpha zz
0.000000	108.23400	97.70127	18.82380
0.250000	108.40480	97.82726	18.83561
0.500000	108.91847	98.20891	18.86943

The following table contains the keywords automatically sent to MOPAC and those you can use to affect this property.

Keyword	Description
POLAR (E=(n1, n2, n3))	Automatically sent to MOPAC to specify the polarizablity routine. n is the starting voltage in eV. The default value is E = 1.0. You can reenter the keyword and another value for n to change the starting voltage.

Keyword	Description
GEO-OK	Automatically sent to MOPAC to override checking of the Z-matrix.
MMOK	Automatically sent to MOPAC to specify Molecular Mechanics correction for amide bonds. Use the additional keyword NOMM to turn this keyword off.

Example 5

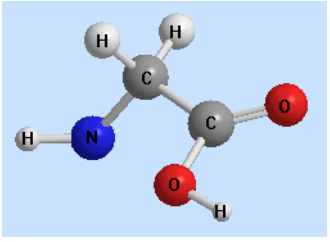
Comparing the Stability of Glycine Zwitterion in Water and Gas Phase

To compare stabilities:

1. From the **File** menu, choose **New Model**.
2. Click the Text Building tool.
3. Click in the model window.

   A text box appears.
4. Type HGlyOH and press the **Enter** key.

   A model of glycine appears.



5. From the **MOPAC Interface** submenu of the **Calculations** menu, choose **Minimize Energy**.
6. On the Theory tab, choose **PM3**.
7. On the Property tab, Ctrl+click **Heat of Formation** and **COSMO Solvation**.
8. Click **Run**.

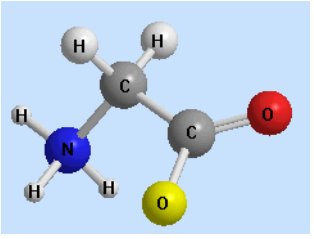
   The results appear in the Messages window.
9. From the **MOPAC Interface** submenu of the **Calculations** menu, choose **Minimize Energy**.
10. On the Property tab, deselect **COSMO Solvation**.
11. Click **Run**.

    The results appear in the Messages window.

To create the zwitterionic form:

1. Click the Text Building tool.
2. Click the **nitrogen**, type "+", then press the **Enter** key.
3. Click the oxygen atom, type "-", then press the **Enter** key.

   The glycine zwitterion is formed.



4. Perform a minimization with and without the COSMO solvation property selected as performed for the glycine model.

The following table summarizes the results of the four analyses.

Form of glycine	ΔH (kcal/mole)	Solvent Accessible Surface Å^2
neutral (H2O)	-108.32861	52.36067
zwitterion (H2O)	-126.93974	52.37133

Form of glycine	ΔH (kcal/mole)	Solvent Accessible Surface Å^2
neutral (gas)	-92.75386	
zwitterion (gas)	-57.83940	

From this data you can reason that the glycine zwitterion is the more favored conformation in water and the neutral form is more favored in gas phase.

Example 6

Hyperfine Coupling Constants for the Ethyl Radical

To build the model:

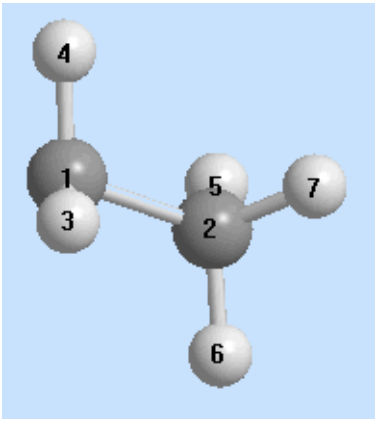
1. From the File menu, choose **New Model**.
2. Click the **Text Building** tool.
3. Click in the model window.

   A text box appears.
4. Type EtH and press the **Enter** key.
5. Click the Select tool.
6. Select **H(8)**.
7. Press the Backspace key.

If you have automatic rectification on, a message appears asking to turn it off to perform this operation.

8. Click **Turn Off Automatic Rectification**.

The Ethyl Radical is displayed.



To perform the HFC computation:

1. From the **MOPAC Interface** submenu of the Calculations menu, choose **Minimize Energy**.
2. On the Theory tab, choose the **PM3** potential function and the **Open Shell (Unrestricted)** wave function.
3. On the Properties tab, choose **Hyperfine Coupling Constants**.
4. Click **Run**.

The unpaired electron in the ethyl radical is delocalized. Otherwise, there would be no coupling constants.

Hyperfine Coupling Constants	
C1	0.02376
C2	-0.00504
H3	-0.02632
H4	-0.02605
H5	0.00350

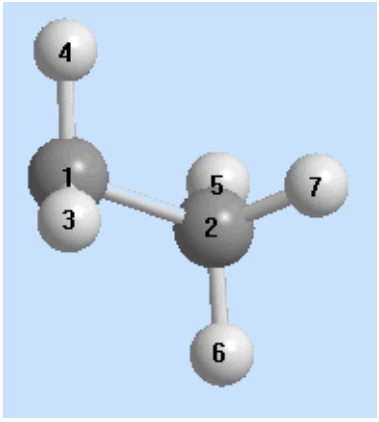
Hyperfine Coupling Constants	
H6	0.05672
H7	0.05479

Example 7

UHF Spin Density for the Ethyl Radical

To calculate the UHF spin density:

1. Create the ethyl radical as described in "Spin Density" on page 189.



2. From the **MOPAC Interface** submenu of the Calculations menu, choose **Minimize Energy**.
3. On the Theory tab, select **PM3**.
4. On the Properties tab, select **Open Shell (Unrestricted)** and **Spin Density**.

The Message window displays a list of atomic orbital spin densities.

The atomic orbitals are not labeled for each value, however, the general rule is shown in the table below (MOPAC only uses s, p_x, p_y and p_z orbitals).

Atomic Orbital Spin Density	A.O.
0.07127	C1 s
0.06739	C1 p_x
0.08375	C1 p_y
0.94768	C1 p_z
-0.01511	C2 S
-0.06345	C2 p_x
-0.01844	C2 p_y
-0.03463	C2 p_z
-0.07896	H3 s
0.07815	H4 s
0.01046	H5 s
0.05488	H6 s
0.05329	H7 s

You can reason from the result shown below that the unpaired electron in the ethyl radical is more localized at $p_{\tilde{z}}$ orbital on C1. Generally, this is a good indication of the reactive site

Example 8

RHF Spin Density for the Ethyl Radical

To calculate the RHF spin density:

1. Create the ethyl radical as described in "Spin Density" on page 189.
2. From the **MOPAC Interface** submenu of the Calculations menu, choose **Minimize Energy**.
3. On the Theory tab, choose **PM3** and **Closed Shell (Restricted)**.
4. On the Properties tab, choose **Spin Density**.

   The Message window displays the total spin densities for each atom (spin densities for all orbitals are totaled for each atom).

NOTE: *You can look in the *.out file for a breakdown of the spin densities for each atomic orbital.*

Total Spin Density

0.90744	C1
0.00644	C2
0.00000	H3
0.00000	H4
0.00001	H5
0.04395	H6
0.04216	H7

You can reason from this result that the unpaired electron in the ethyl radical is more localized on C1. Generally, this is a good indication of the reactive site.

Chapter 11: ULTRA Gaussian Computations

Gaussian Overview

The following procedures describe the graphical user interface (GUI) Chem3D provides for users of Gaussian 03W. For information about how to use Gaussian, see the documentation supplied by Gaussian, Inc., makers of the application.

Gaussian 03W is not included with Chem3D, but can be purchased separately from CambridgeSoft. You can use the Online menu command Browse ChemStore.com to link directly to the website.

Gaussian 03

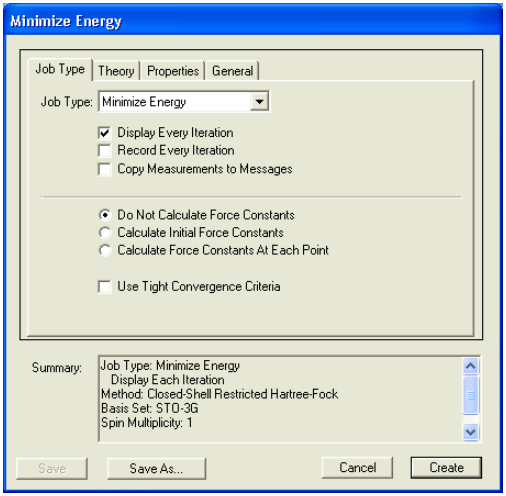
Gaussian 03W is a powerful computational chemistry application including both *ab initio* and semiempirical methods. Gaussian is a command-line application that requires a user to type text-based commands and data instead of selecting graphical objects and menu items. Chem3D serves as a front-end GUI for Gaussian 03W, enabling you to create and run Gaussian jobs in Chem3D. The model in the Chem3D window transparently provides the data for Gaussian computations. Menus and dialog boxes replace the many Gaussian commands, although Chem3D preserves the option to use them for less common and advanced computations.

Minimize Energy

To perform a minimize energy computation on a molecule:

From the Calculations menu, point to Gaussian and choose Minimize Energy.

The Minimize Energy dialog box appears.



The Job Type Tab

The Job Type tab of the dialog box defaults to Minimize Energy when you select Minimize Energy from the menu. Job Type can be changed to Compute Properties from within this tab.

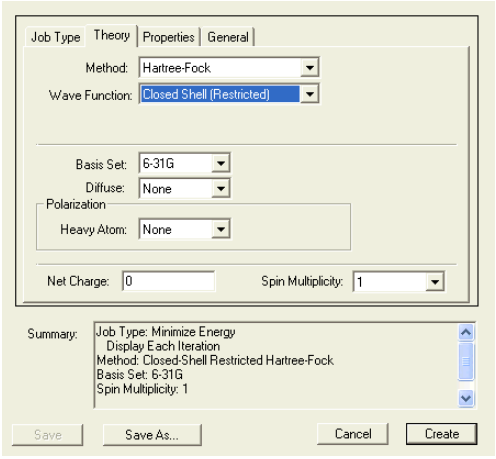
Select the appropriate options:

If you want to ...	Then select ...
watch the minimization process "live" at each iteration in the calculation	Display Every Iteration *NOTE: Displaying or recording each iteration adds significantly to the time required to minimize the structure.*

If you want to ...	Then select ...
record each iteration as a frame in a movie for later replay	Record Every Iteration
view the value of each measurement in the Measurement table	Copy Measurements to Output
calculate the second derivative matrix determined from atomic radii and a simple valence force field. This is the Gaussian default initial guess.	Do Not Calculate Force Constants
calculate the initial force constant at the current level of theory. Corresponds to the Gaussian keyword Opt = CalcFC	Calculate Initial Force Constants
calculate a new force constant at every point in the minimization. Corresponds to the Gaussian keyword Opt=CalcAll.	Calculate Force Constants At Each Point
calculate using the equivalent to the Gaussian keyword Opt=Tight	Use Tight Convergence Criteria

The Theory Tab

Use the Theory tab to specify the combination of basis set and particular electronic structure theory referred to in Gaussian documentation as the model chemistry. By default, this tab is optimized for setting up *ab initio* computations.



To set the Theory specifications:

1. Select the appropriate Method.

   NOTE: *To use a Method or Basis Set that is not on the list, type it in the Additional Keywords section on the General page. For more information, see "The General Tab" on page 201.*

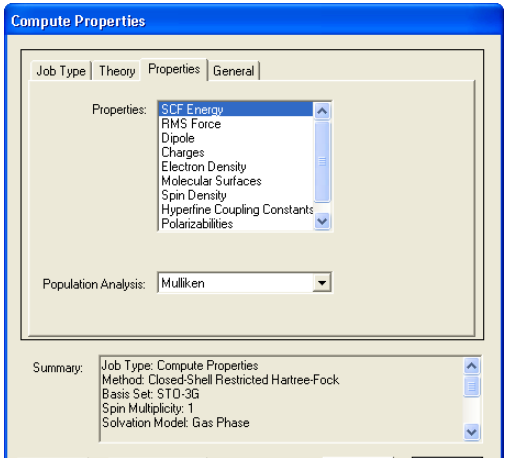
2. Select the wave function to use: Closed Shell (Restricted), Open Shell (Unrestricted), or Restricted Open Shell.
3. Select the Basis Set.
4. Select the Diffuse function to add to the basis set.
5. Select the Polarization Heavy Atom.

   If you select a Heavy Atom function, also choose an H option.

6. Select a Spin Multiplicity value between one and 10.

The Properties Tab

The Properties tab allows you to select the properties and charges to calculate from the minimized structure.

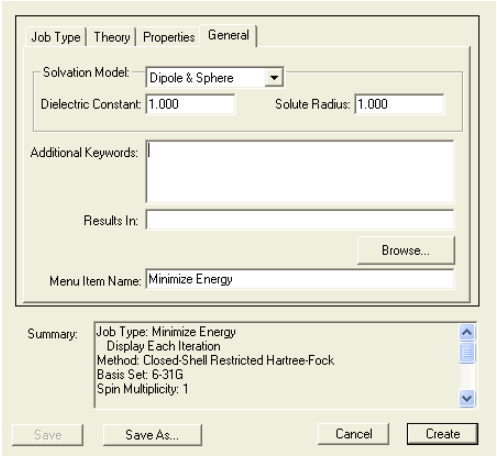


To set the properties and charges:

7. From the Properties list, select the properties to calculate.
8. From the Population Analysis list, select the method to compute atomic charges:
   - Mulliken population analysis
   - Electrostatic potential-derived charges according to the CHelp, CHelpG, and Merz-Singh-Kollman schemes
   - Natural Bond Order analysis (NBO)
   - Analysis according to the *Theory of atoms in molecules* by Bader *et al.* (Atoms In Molecules).

The General Tab

The General tab allows you to customize the calculation for the model.



To specify the general settings:

1. From the Solvation Model list, choose a solvation model:
   - Gas Phase
   - Onsager Model (Dipole & Sphere)
   - Tomasi's PCM Model (PCM Model)
   - Isodensity Model (I-PCM Model)
   - Self-consistent Isodensity Model (SCI-PCM Model)
2. Enter values for:
   - Dielectric Constant, ε, for the solvent
   - Solute Radius
   - Points per Sphere
   - Isodensity

   as appropriate

   NOTE: *No value entry boxes appear for gas-phase computations.*
3. Type Gaussian keywords in the Additional Keywords text box for access to less common or more advanced functionality.

In the Results In text box, specify the path to the directory where results are stored by typing or browsing.

Save a customized job to appear as a Gaussian submenu item as follows:

1. In the Menu Item Name text box, type the name of the job description.
2. Click Save As.

   The Save dialog box appears.
3. Browse to the Gaussian Job folder in the \Chem3D\C3D Extensions folder.

   NOTE: *The file must be saved in the Gaussian Job folder in order for it to appear in the menu.*
4. Select the file type to save. For more information, see "Job Description File Formats" on page 202.
5. Click Save.

Job Description File Formats

Job description files are like Preferences files; they store the settings of the dialog box. You may save the file as either a .jdf or a .jdt type. You modify and save .jdf files more easily than .jdt files.

.jdt Format

The .jdt format is a template format intended to serve as a foundation from which other job types may be derived. The Minimize Energy and Compute Properties job types supplied with Chem3D are examples of these. To discourage modification of these files, the Save button is deactivated in the dialog box of a template file.

.jdf Format

The .jdf format is a file format for saving job descriptions. Clicking Save within the dialog box saves modifications without the appearance of a warning or confirmation dialog box.

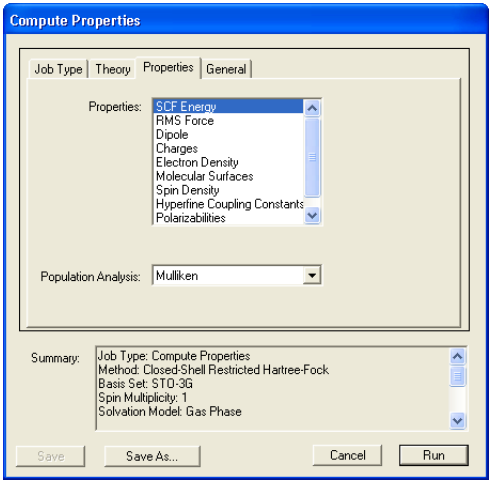
Saving either format within the Gaussian Job folder adds it to the Gaussian submenu for convenient access.

Computing Properties

To specify the parameters for computations to predict properties of a model:

- From the Calculations menu, point to Gaussian and choose Compute Properties.

  The Compute Properties dialog box appears and displays the Properties tab with the top property of the menu preselected.



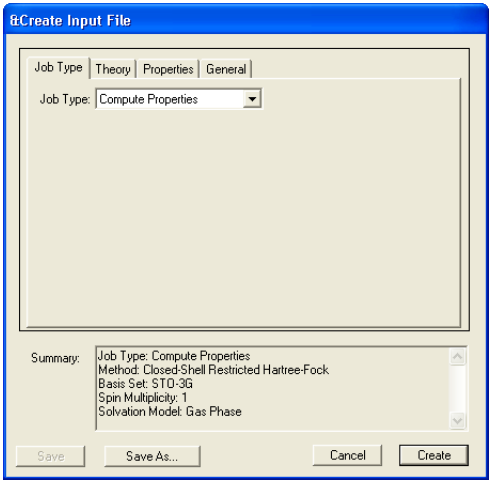
Creating a Gaussian Input File

A Gaussian Input file contains the coordinates and geometry of the model and the Gaussian keywords taken from the settings of the dialog box.

To create a Gaussian Input file:

1. From the Gaussian submenu, choose Create Input File.

   The Create Input File dialog box appears.



2. Click Create.

   An input file saves in Gaussian's native .GJF format.

NOTE: *The .GJF Gaussian Input File is not the same as the .GJC Gaussian Input File. The .GJC file stores only the model coordinates and not the Gaussian keywords specifying computational parameters.*

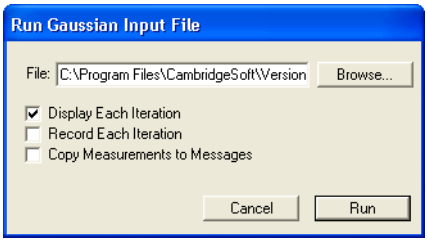
Running a Gaussian Input File

If you have a previously created .GJF Gaussian input file, you can run the file from within Chem3D.

To run a Gaussian input file:

1. From the Gaussian submenu, choose Run Input File.

   The Run Gaussian Input file dialog box appears.



2. Type the full path of the Gaussian file or Browse to location.
3. Select the appropriate options.

If you want to ...	Then click ...
watch the minimization process "live" at each iteration in the calculation	Display Every Iteration *NOTE: Displaying or recording each iteration adds significantly to the time required to minimize the structure.*
record each iteration as a frame in a movie for later replay	Record Every Iteration
track a particular measurement	Copy Measurements to Output

4. Click Run.

   A new model window is created and the initial model appears. The Gaussian job runs and the results will appear.

   All properties requested for the job appear in the *.out file. Only iteration messages appear for Gaussian Input File jobs.

Repeating a Gaussian Job

After you perform a Gaussian calculation, you can repeat the job as follows:

1. From the Gaussian submenu, choose Repeat [*name of computation*].

   The appropriate dialog box appears.
2. Change parameters if desired and click Run.

   The computation proceeds.

Running a Gaussian Job

Chem3D enables you to select a previously created Gaussian job description file (.jdf). The .jdf file can be thought of as a set of Settings that apply to a particular dialog box.

You can create a .jdf file from the dialog box of any of the Gaussian calculations (Minimize Energy, Optimize to Transition State) by clicking Save As after all Settings for the calculation have been set. For more information about .jdf files see "Job Description File Formats" on page 126.

To run a Gaussian job:

1. From the Gaussian submenu, choose Run Gaussian Job.

   The Open dialog box appears.
2. Select the file to run.

   The dialog box corresponding to the type of job (Minimize Energy, Compute Properties, and so on.) saved within the file appears.
3. Click Run.
4.

Chapter 12: SAR Descriptors

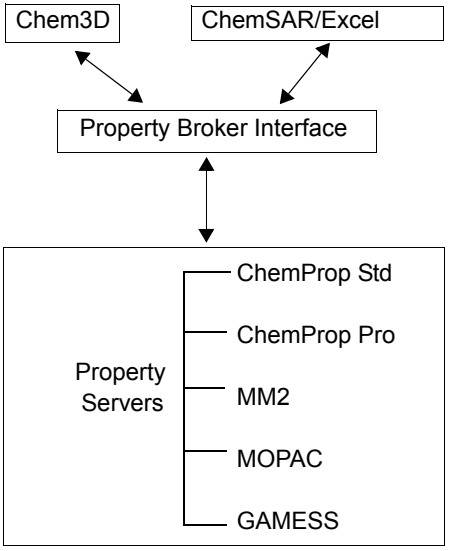
SAR Descriptor Overview

Chem3D provides a set of physical and chemical property predictors. These predictors, which help predict the structure-activity relationship (SAR) of molecules, are referred to as SAR descriptors in this user's guide. These descriptors are also available in ChemSAR/Excel.

Chem3D Property Broker

The Chem3D Property Broker provides an interface in Chem3D and ChemSAR/Excel that allows you to calculate properties using many calculation methods provided by various Property Server components.

The components of the Property Broker-Server architecture are illustrated below:



ChemProp Std Server

The ChemProp Std Server enables you to calculate the following structural properties:

Property	Description
Connolly Solvent Accessible Surface Area (Angstroms^2)	The locus of the center of a spherical probe (representing the solvent) as it is rolled over the molecular model.

Property	Description
Connolly Molecular Surface Area (Angstroms^2)	The contact surface created when a spherical probe sphere (representing the solvent) is rolled over the molecular model.
Connolly Solvent-Excluded Volume (Angstroms^3)	The volume contained within the contact molecular surface.
Exact Mass (g/mole)	The exact molecular mass of the molecule, where atomic masses of each atom are based on the most common isotope for the element.
Formal Charge (electrons)	The net charge on the molecule.
Molecular Formula	The molecular formula showing the exact number of atoms of each element in the molecule.
Molecular Weight (atomic mass units)	The average molecular mass of the structure, where atomic masses are based on the weighted average of all isotope masses for the element.
Ovality	The ratio of the Molecular Surface Area to the Minimum Surface Area. The Minimum Surface Area is the surface area of a sphere having a volume equal to the Solvent-Excluded Volume of the molecule. Computed from the Connolly Molecular Surface Area and Solvent-Excluded Volume properties.
Principal Moments of Inertia (X, Y, Z) (grams/mole Angstroms^2)	The Moments of Inertia when the Cartesian coordinate axes are the principal axes of the molecule.

The surface area and volume calculations are performed with Michael Connolly's program for computing molecular surface areas and volume (M. L. Connolly. The Molecular Surface Package. *J. Mol. Graphics* **1993,** *11*).

For the latest information about the Connolly programs and definitions of the area and volume properties, see the following web site:
http://connolly.best.vwh.net/

NOTE: *The default Probe Radius used in the calculation is 1.4 angstroms. You can change the Probe Radius value in the Parameters dialog box.*

The Principal Moments of Inertia are the diagonal elements of the inertia tensor matrix when the Cartesian coordinate axes are the principal axes of the molecule, with the origin located at the center of

mass of the molecule. In this case, the off-diagonal elements of the inertia tensor matrix are zero and the three diagonal elements, I_{xx}, I_{yy}, and I_{zz} correspond to the Moments of Inertia about the X, Y, and Z axes of the molecule.

ChemProp Pro Server

ULTRA

CS ChemProp Pro server allows you to predict the following physical and thermodynamic properties of molecules.

NOTE: *Fragmentation methods and literature values are used for these calculations. Use the Full Report property to view references for the methods.*

Property	Description
Boiling Point (Kelvin)	The boiling point for the structure at 1 atm.
Critical Temperature (Kelvin)	The temperature (T_c) above which the gas form of the structure cannot be liquefied, no matter the applied pressure.
Critical Pressure (bar)	The minimum pressure (P_c) that must be applied to liquefy the structure at the critical temperature.
Critical Volume (cm^3/mole)	The volume occupied (V_c) at the compound's critical temperature and pressure.
Full Report	A detailed list of information used for performing the calculations, including additional properties and literature references used. Results for other fragmentation methods are included.
Heat of Formation (kcals/mole)	The heat of formation (ΔH_f) for the structure at 298.15 K and 1 atm.
Henry's Law Constant (unitless)	The inverse of the logarithm of Henry's law constant [-log(H)].
Ideal Gas Thermal Capacity (J/[mole K])	The constant pressure (1 atm) molar heat capacity at 298.15 K for an ideal gas compound.
LogP	The logarithm of the partition coefficient for n-octanol/water.
Melting Point (Kelvin)	The melting point for the structure at 1 atm.
Molar Refractivity (cm^3/mole)	The molar refraction index.
Standard Gibbs Free Energy (kJ/mole)	The Gibbs free energy (ΔG) for the structure at 298.15 K and 1 atm.

Property	Description
Vapor Pressure (Pa)	The vapor pressure for the structure at 25° C.
Water Solubility at 25° C (mg/L)	Prediction of the water solubility of the structure.

Limitations

Property prediction using CS ChemProp Pro has following limitations:

- Single molecules with no more than 100 atoms.
- Literature values for Partition Coefficients (LogP) and Henry's Law Constant are not available for all molecules.
- Some atom arrangements are not parameterized for the fragmentation methods used to calculate the properties.

Because of these limitations, the property prediction fails for some molecules.

Error Messages

If ChemProp Pro fails, one of the following error messages appears:

Error Message	Cause
Unparametrized fragment	A fragment in the molecule is unrecognized so no parameters exist for the property calculation.
Out of memory failure	There is insufficient memory for the calculation.
Data not in database	The literature values for this property are not in the database.
Bad MDL Molfile format	The molecule is too large or complex, causing bad input data to be generated.
Invalid aggregate	A fragment in the molecule is unrecognized or there is more than one disjointed molecule or fragment.
Too many molecules	There is more than one molecule.
Too many atoms	There are more than 100 atoms.
exceeded MDL Molfile size limit	The input data generated for this molecule exceeds the maximum size limit.

[ULTRA] MM2 Server

The MM2 server computes property predictions using the methods of molecular mechanics. For more information on MM2, see "Molecular Mechanics Theory in Brief" on page 135 and 'MM2 and MM3 Computations"

The MM2 server provides the following property calculations:

Property	Description
Bending Energy (kcal/mol)	The sum of the angle-bending terms of the force-field equation.
Charge-Charge Energy (kcal/mol)	The sum of the electrostatic energy representing the pairwise interaction of charged atoms.
Charge-Dipole Energy (kcal/mol)	The sum of the electrostatic energy terms resulting from interaction of a dipole and charged species.
Dipole Moment (Debye)	Molecular dipole moment.
Dipole-Dipole Energy (kcal/mol)	The sum of the electrostatic energy terms resulting from interaction of two dipoles.
Non-1,4 van der Waals Energy (kcal/mol)	The sum of pairwise van der Waals interaction energy terms for atoms separated by more than 3 chemical bonds.
Stretch-Bend Energy (kcal/mol)	The sum of the stretch-bend coupling terms of the force-field equation.
Torsion Energy (kcal/mol)	The sum of the dihedral bond rotational energy term of the force-field equation.
Total Energy (kcal/mol)	The sum of all terms the the force-field equation.
van der Waals Energy (kcal/mol)	The sum of pairwise van der Waals interaction energy terms for atoms separated by exactly 3 chemical bonds.

MOPAC Server ULTRA

The MOPAC server calculates property predictions based on semi-empirical computational methods. For more information, see "The Semi-empirical Methods" on page 146 and "Running MOPAC Jobs" on page 178

The MOPAC server provides the following property calculations:

Property	Description
Alpha Coefficients	First order polarizability coefficients.
Beta Coefficients	Second order polarizability coefficients.
Dipole (Debye)	Molecular dipole moment.

Property	Description
Electronic Energy (298 K) (eV at 0^{o} Celsius)	The total electronic energy.
Gamma Coefficients	Third order polarizability coefficients.
HOMO Energy (eV)	Energy of the highest occupied molecular orbital.
LUMO Energy (eV)	Energy in of the lowest unoccupied molecular orbital.
Repulsion Energy (eV)	Total core-core internuclear repulsion between atoms.
Symmetry	Point group symmetry.
Total Energy (eV)	The sum of the MOPAC Electronic Energy and the MOPAC Repulsion Energy.

GAMESS Server ULTRA

GAMESS uses *ab initio* computational methods to compute property predictions. For more information, see "" and "."

The GAMESS server provides the following property calculations:

Property	Description
Dipole Moment (Debye)	Molecular dipole moment.
HOMO Energy (eV)	Energy of the highest occupied molecular orbital.
LUMO Energy (eV)	Energy of the lowest unoccupied molecular orbital.
Repulsion Energy Energy (eV)	Total core-core internuclear repulsion between atoms.
Total Energy (eV)	The total energy of the molecule.

Chapter 13 : ULTRA GAMESS Computations

GAMESS Overview

The General Atomic and Molecular Electronic Structure System (GAMESS) is a general *ab initio* quantum chemistry package maintained by the Gordon research group at Iowa State University. It computes wavefunctions using RHF, ROHF, UHF, GVB, and MCSCF. CI and MP2 energy corrections are available for some of these.

GAMESS is a command-line application, which requires a user to type text-based commands and data. Chem3D serves as a front-end graphical user interface (GUI), allowing you create and run GAMESS jobs from within Chem3D.

Installing GAMESS

You must download and install the GAMESS application separately.

You can download the GAMESS application and documentation from the following web site:

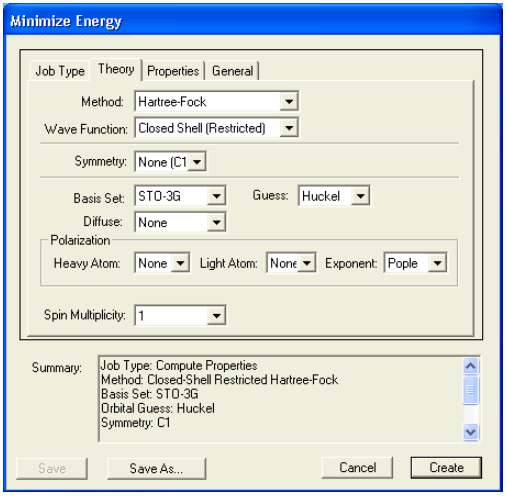
http://www.msg.ameslab.gov/GAMESS/GAMESS.html

Minimize Energy

To perform a GAMESS Minimize Energy computation on a model:

1. From the Calculations menu, point to Gamess and choose Minimize Energy.

   The Minimize Energy dialog box appears with the Theory tab displayed.



2. Use the tabs to customize your computation. See the following sections for details.
3. Click Run.

The Theory Tab

Use the Theory tab to specify the combination of basis set and particular electronic structure theory. By default, this tab is optimized for setting up *ab initio* computations.

For more detailed information, see the $BASIS section of the GAMESS documentation.

To specify the calculation settings:

1. From the Method list, choose a method.
2. From the Wave Function list, choose a function.
3. From the Basis Set list, choose the basis set.

> ***NOTE:*** *To use a Method or Basis Set that is not on the list, type it in the Additional Keywords section on the General tab. For more information, see "Specifying the General Settings" on page 213.*

4. From the Diffuse list, select the diffuse function to add to the basis set.
5. Set the Polarization functions.

   If you select a function for Heavy Atom, also select an H option.
6. Select a Spin Multiplicity value between 1 and 10.

The Job Type Tab

Use the Job Type tab to set options for display and recording results of calculations.

To set the job type options:

1. In the Minimize Energy dialog box, click the Job Type tab.
2. Select the appropriate options:

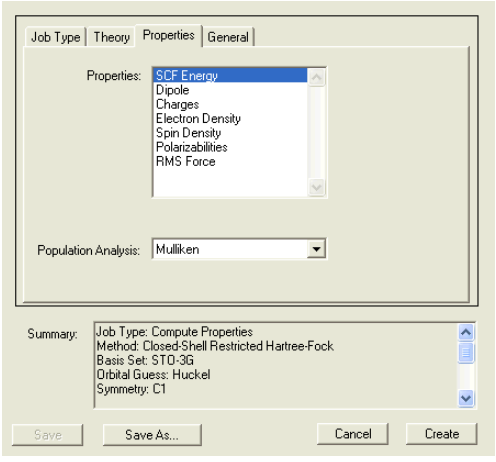
If you want to ...	Then click ...
watch the minimization process live at each iteration in the calculation	Display Every Iteration *NOTE: Displaying or recording each iteration adds significantly to the time required to minimize the structure.*
record each iteration as a frame in a movie for later replay	Record Every Iteration
view the value of each measurement in the Measurement table	Copy Measurements to Output
calculate using the equivalent to the Gamess keyword Opt=Tight	Use Tight Convergence Criteria

Specifying Properties to Compute

Use the Properties tab to specify which properties are computed. The default Population Analysis type is Mulliken.

To specify properties:

1. In the Minimize Energy dialog box, click Properties.



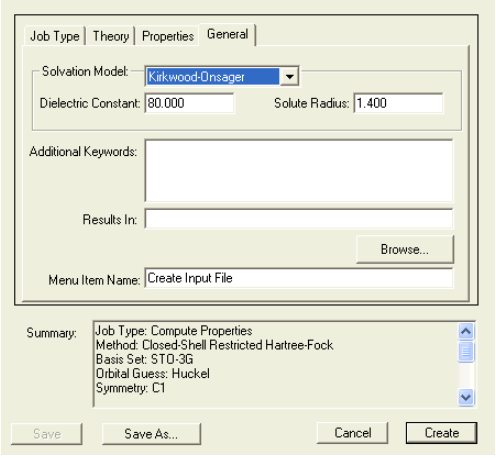
2. On the Properties tab, set the following options:
   - Select the properties to calculate
   - Select the Population Analysis type

Specifying the General Settings

Use the General tab to customize the calculation to the model.

To set the General settings:

1. In the Minimize Energy dialog box, click General.



2. On the General tab, set the following options:
   - Select the Solvation model.
   - Type the dielectric constant for the solvent. The box does not appear for gas-phase computations.
   - In the Results In box, type or browse to the path to the directory where results are stored.
   - If desired, add GAMESS keywords to the Additional Keywords dialog box.

Saving Customized Job Descriptions

After you customize a job description, you can save it as a Job Description file to use for future calculations.

For more information, see "Job Description File Formats" on page 126.

To save a GAMESS job:

1. On the General tab, type the name of the file in the Menu Item Name text box.

   The name you choose will appear in the GAMESS menu.
2. Click Save As.

   The Save dialog box appears.
3. Open the folder \Chem3D\C3D Extensions\GAMESS Job.

   NOTE: *You must save the file in the GAMESS Job folder for it to appear in the menu.*
4. Select the .jdf or .jdt file type.
5. Click Save.

   Your custom job description appears in the GAMESS menu.

Running a GAMESS Job

If you have a previously created an .inp GAMESS job file, you can run the file in Chem3D.

To run the job file:

1. From the Calculations menu, point to Gamess and choose Run GAMESS Job.

   The Open dialog box appears.
2. Type the full path of the GAMESS file or Browse to location.

3. Click Open.

   The appropriate dialog box appears.

4. Change settings on the tabs if desired.
5. Click Run.

   A new model window is created and the initial model will appear. The GAMESS job runs and the results appear.

   Properties requested for the job appear in the *.out file. Only iteration messages will appear.

Repeating a GAMESS Job

After a GAMESS computation has been performed, you can repeat it using the GAMESS menu.

To repeat a GAMESS job:

1. From the Calculations menu, point to Gamess and choose Repeat [*name of computation*].

   The appropriate dialog box appears.

2. Change parameters if desired and click Run.

   The computation proceeds.

Chapter 14: SAR Descriptor Computations

Overview

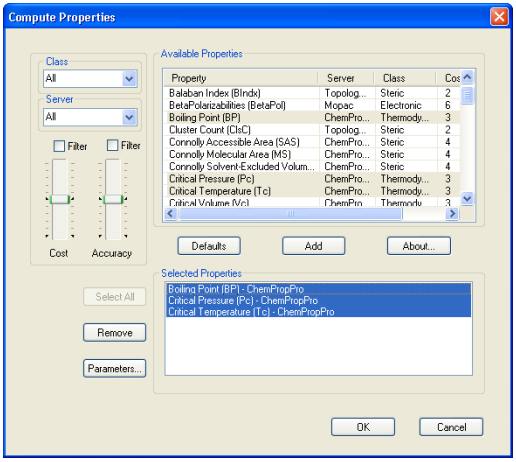
Chem3D performs property prediction calculations. These computed properties are the descriptors that may be used to estimate the structure-activity relationship (SAR) of molecules.

Selecting Properties To Compute

To select properties for computation:

1. From the Calculations menu, choose Compute Properties.

   The Compute Properties dialog box appears.



2. Set appropriate values for the Class, Server, Cost, and Quality filters.

   For more information, see "Property Filters" on page 215.

3. From the list of Available Properties, select the properties to calculate.

4. Click Add.

   The properties you select appear in the Selected Properties list.

NOTE: *Some properties may not be computed for a particular model because of the limitations of standard computational methods.*

Sorting Properties

To sort the properties in the Property and Method columns:

- Click the column heading.

  The items in the columns are sorted.

Removing Selected Properties

To remove properties from the Selected Properties list:

1. Select the properties to delete or click Select All to select all the properties.
2. Click Remove.

   The properties are removed from the list.

Property Filters

Property filters allow you to select what properties appear in the Available Properties list.

The property filters are:

- **Class**—limits the list of available properties to types calculations that you specify.

- **Server**—limits the list of available properties to those properties computed by the servers you specify.
- **Cost**—represents the maximum acceptable computational cost. It limits the list of available properties to those which are less than or equal to the computational cost specified.
- **Quality**—represents the minimum acceptable data quality. It limits the list of available properties to those with quality greater than or equal to the quality specified.

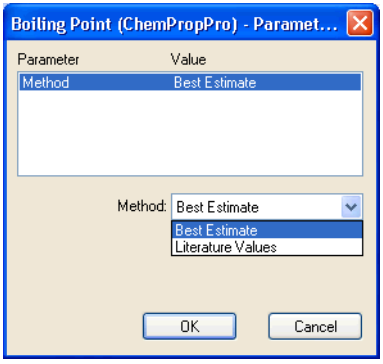
Setting Parameters

If a property has one or more parameters that affect the result of the calculation, you can specify the values or calculation method of those parameters. If several properties have the same parameters, you can change the parameters simultaneously.

To change a parameter:

1. Select the property or properties in the Selected Properties list.
2. Click Parameters.

   One of the following dialog boxes appears, depending on the selected parameters.



3. Edit the value or select the method.
4. Click OK.

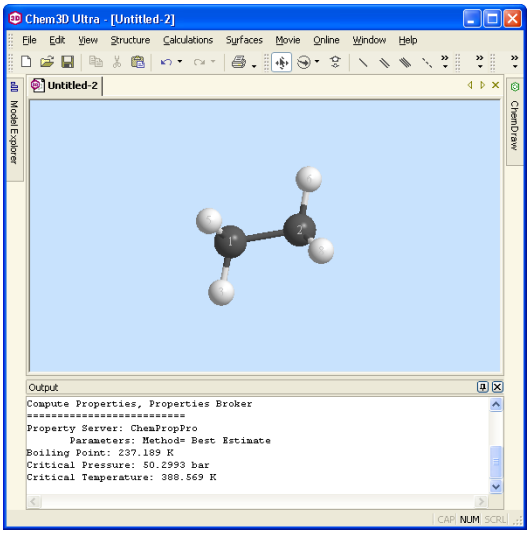
   The new value is set.

Results

To perform the calculation:

- Click OK.

  Chem3D performs the calculation and displays the results in the Output window.



Chapter 15: ULTRA ChemSAR/Excel

Overview

ChemSAR/Excel is a Chem3D Ultra addin for Microsoft Excel. ChemSAR/Excel enables you to calculate the physiochemical properties (descriptors) for a set of structures in an Excel worksheet.

ChemSAR/Excel provides statistical tools to help identify trends in the calculated properties and correlate the data.

To run ChemSAR/Excel, you must have the following installed on your computer:

- Chem3D Ultra.
- ChemFinder.
- MS Excel 2000, 2003, or XP.

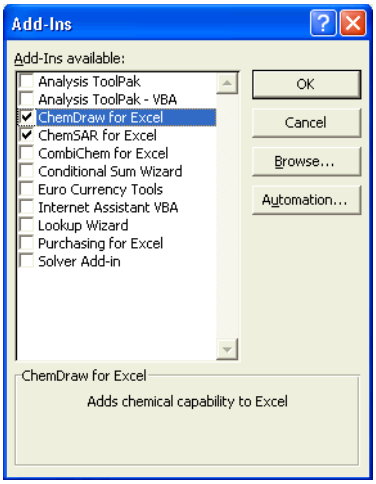
Configuring ChemSAR/Excel

When you install Chem3D or ChemOffice, the ChemSAR/Excel add-in is automatically installed.

To start ChemSAR/Excel:

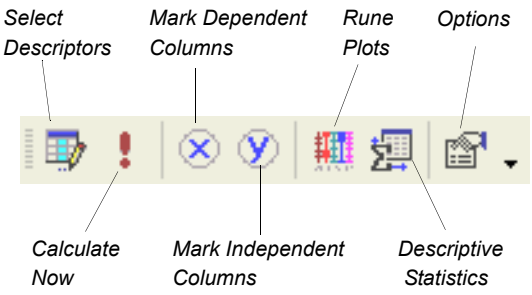
1. Open MS Excel.
2. From the Tools menu, choose Add-Ins.

   The Add-Ins dialog box appears.



3. Click ChemDraw for Excel and ChemSAR for Excel.
4. Click OK.

   The ChemSAR/Excel toolbar appears.



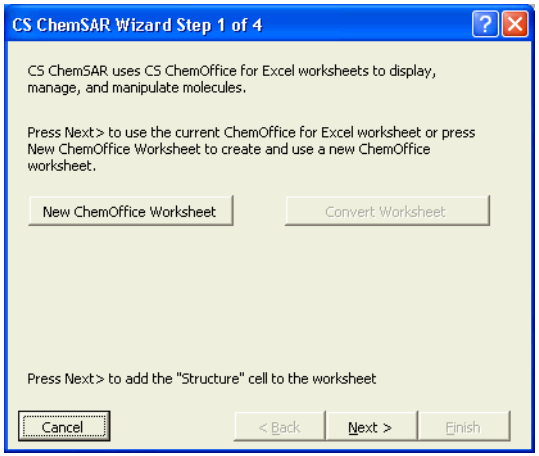
The ChemSAR/Excel Wizard

The ChemSAR/Excel wizard leads you through the steps required to perform property calculations on a set of molecules.

To perform property calculations using the ChemSAR/Excel Wizard:

1. From the ChemOffice menu, point to ChemSAR, then choose Wizard.

   The Step 1 of 4 dialog box appears.


CS ChemSAR Wizard Step 1 of 4
CS ChemSAR uses CS ChemOffice for Excel worksheets to display, manage, and manipulate molecules.
Press Next> to use the current ChemOffice for Excel worksheet or press New ChemOffice Worksheet to create and use a new ChemOffice worksheet.
New ChemOffice Worksheet
Convert Worksheet
Press Next> to add the "Structure" cell to the worksheet
Cancel
< Back
Next >
Finish

2. Select the appropriate option:

If you want to	Then click
create a new ChemOffice worksheet	New ChemOffice Worksheet
convert the current Excel worksheet to a ChemOffice worksheet	Convert Worksheet

> ***NOTE:*** *If you are already in a ChemOffice worksheet, the "Convert" button is grayed out and you can immediately click "Next".*

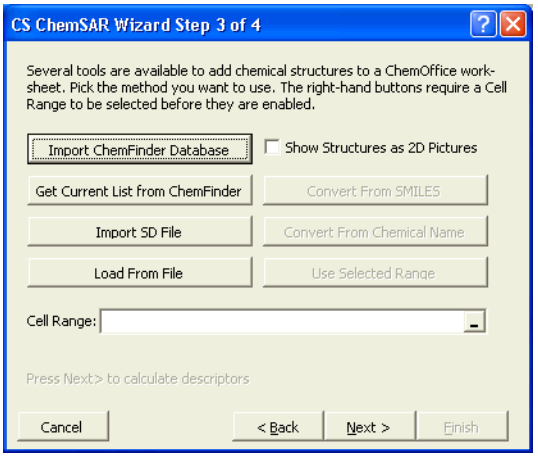
3. Click Next.

   The Step 2 of 4 dialog box appears.

CS ChemSAR Wizard Step 2 of 4
Select a cell to label "Structure"; molecules will be placed in this column below this cell; column labels for calculated descriptors will be placed in this row to the right of this cell
"Structure" Cell:
$A$1
Press Next> to add structures to the worksheet
Cancel
< Back
Next >
Finish

4. Click in the cell that will be the heading cell for the structure column, or type in a cell reference.
5. Click Next.

   The Step 3 of 4 dialog box appears.

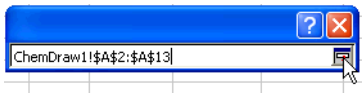

CS ChemSAR Wizard Step 3 of 4
Several tools are available to add chemical structures to a ChemOffice worksheet. Pick the method you want to use. The right-hand buttons require a Cell Range to be selected before they are enabled.
Import ChemFinder Database
Show Structures as 2D Pictures
Get Current List from ChemFinder
Convert From SMILES
Import SD File
Convert From Chemical Name
Load From File
Use Selected Range
Cell Range:
Press Next> to calculate descriptors
Cancel
< Back
Next >
Finish

   The buttons on the right are active when you use a range of cells in your worksheet.

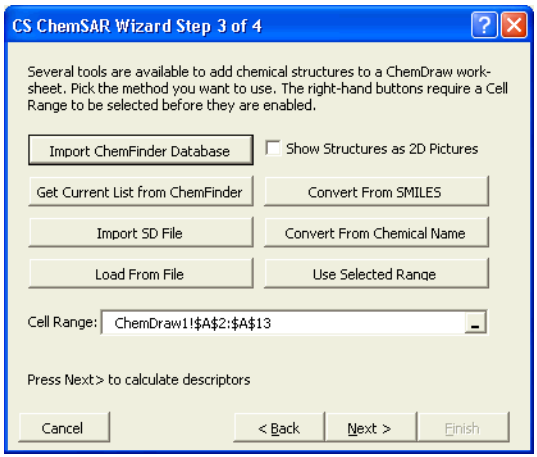
   To select a range of cells:

   a. Click the minus sign at the right end of the Cell Range box. A selection box appears.
   b. Drag the range of cells you want to include.

c. Click the icon at the right of the selection box.



The range is entered and the buttons are active as shown below.

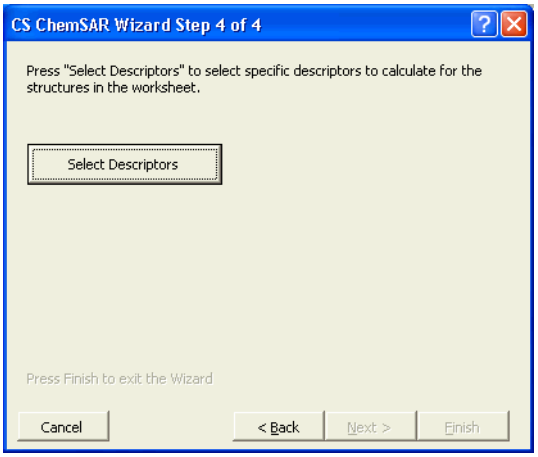

CS ChemSAR Wizard Step 3 of 4
Several tools are available to add chemical structures to a ChemDraw worksheet. Pick the method you want to use. The right-hand buttons require a Cell Range to be selected before they are enabled.
Import ChemFinder Database
Show Structures as 2D Pictures
Get Current List from ChemFinder
Convert From SMILES
Import SD File
Convert From Chemical Name
Load From File
Use Selected Range
Cell Range:
ChemDraw1!$A$2:$A$13
Press Next> to calculate descriptors
Cancel
< Back
Next >
Finish

6. To display graphics of your structures in the worksheet, choose Show Structures As 2D Pictures.
7. Select the appropriate option:

If you want to	Then
use data from a ChemFinder database	a. Click Import ChemFinder Database. b. In the Import Table dialog box choose the database and click Open.
use an active ChemFinder hit list	a. Click Get Current List from ChemFinder. b. Click Yes
import a structure data file into the ChemFinder worksheet	a. Click Import SD File. b. In the Importable dialog box choose the database and click Open.
import a file of one of the following format types: .CDX, .MOL, .SKC, .f1d, .f1q, or .RXN.	a. Click Load from File. b. In the Choose Molecule to Load dialog box, choose the file.
use structures entered as SMILES strings.	a. Select the strings to include. b. Click Convert From SMILES.
use structures entered as text.	a. Select the text to include. b. Click Convert From Chemical Name.
use specific structures in worksheet	a. Type the range of cells containing the structures to use. b. Click Use Selected Range.

8. Click Next.

The Step 4 of 4 dialog box appears.


CS ChemSAR Wizard Step 4 of 4
Press "Select Descriptors" to select specific descriptors to calculate for the structures in the worksheet.
Select Descriptors
Press Finish to exit the Wizard
Cancel
< Back
Next >
Finish

9. Click Select Descriptors.
10. In the Select Descriptors dialog box, select the appropriate descriptors.

    For more information on using the Select Descriptors dialog box, see "Selecting ChemSAR/Excel Descriptors" on page 220.
11. Click Finish.

    The calculations are performed and the results appear in the worksheet.

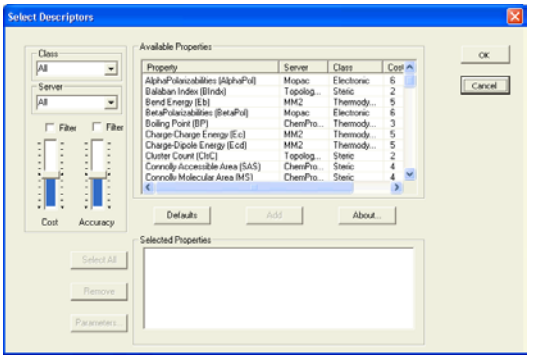
Selecting ChemSAR/Excel Descriptors

The Select Descriptors dialog box allows you to specify which physical properties to calculate for your worksheet. Properties are calculated for entire molecules. If you want to calculate the properties of a molecule fragment, you must add that fragment to your worksheet.

To select descriptors:

1. From the ChemOffice menu, point to ChemSAR, then choose Select Descriptors, or click the Select descriptors icon .

The Select Descriptors dialog box appears:



2. Select the calculation type from the Class drop-down list.
3. Select the computational model from the Server drop-down list.
4. Use the Cost and Accuracy sliders to set the appropriate ratio.

    The greater the cost number, the greater the time it takes for the calculation.

    The greater the accuracy number, the greater the accuracy of method used to perform the calculations.
5. Select the properties to calculate and click Add.
6. To delete a property from the list, click Remove.
7. To view the calculation method of a property, select it and click Parameters.
8. Click OK.

    The calculations are performed.

Adding Calculations to an Existing Worksheet

When you add structures to a worksheet that already has calculated properties, you can calculate the properties for only the added structures without recalculating the entire worksheet.

To calculate properties for added structures:

1. In a worksheet with calculated properties, add the structures for which you want to calculate properties.
2. Click Calculate Now .

   The properties are calculated and added to the worksheet.

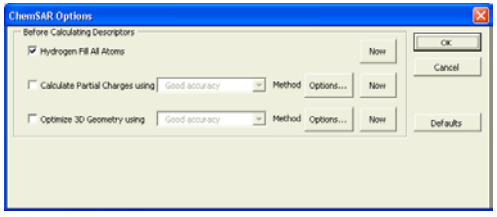
Customizing Calculations

You can use the ChemSAR/Excel Options dialog box to customize a calculation by changing the default settings.

To change the defaults:

1. From the ChemOffice menu point to ChemSAR, then choose Options; or click the Options icon .

   The ChemSAR/Excel Options dialog box appears.



2. To populate any unfilled valences with hydrogen atoms, select Hydrogen Fill All Atoms.
3. To customize the partial charge calculation, click Calculate Partial Charges using.
   d. Select a type of method from the drop-down list.
   e. To further customize the calculation, click Options and then select a Charge Method and Theory to use.
   f. Click Use Custom Settings.
4. To customize the how the 3D geometry is optimized, select Optimize 3D Geometry using.
   g. Select a type of method from the drop-down list.
   h. To further customize the calculation, click Options and then select a Optimization Method, Theory, and RMS Gradient to use.
   i. Click Use Custom Settings.
5. Do one of the following:

To perform the calculation on ...	Click ...
a selected molecule	Now
the entire worksheet	OK

Calculating Statistical Properties

ChemSAR/Excel allows you to calculate the following statistical properties:

- Descriptive Statistics
- Correlation matrix
- Rune Plot

Descriptive Statistics

ChemSAR/Excel calculates the following statistics for every column in the data set:

- Mean
- Minimum
- Maximum
- Range
- Count
- Sum
- Standard deviation
- Median

To perform the statistical calculations:

- From the ChemOffice menu point to ChemSAR, then choose Descriptive Statistics; or click the Statistics icon .

  The results are added as a separate worksheet.

Correlation Matrix

ChemSAR/Excel calculates scatter plots for each property to every other property.

To calculate the correlation matrix:

- From the ChemOffice menu point to ChemSAR, then choose Correlation Matrix.

  The results are displayed on a separate worksheet. correlating cells are colored.

Rune Plots

Rune plots are used to compare data and visualize how normally the data is distributed. The data is transformed on a scale of zero to one. Each data set is then plotted next to each other. You can then identify data sets that are not normally distributed and exclude them from any further calculation.

To create Rune plots:

- From the ChemOffice menu point to ChemSAR, then choose Rune Plots; or click the Rune Plots icon .

  The plot is added as a separate worksheet.

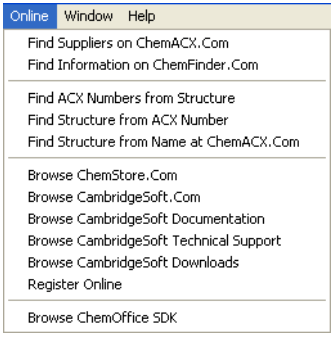
Appendix A: Accessing the CambridgeSoft Web Site

Online Menu Overview

The ChemOffice **Online** menu gives you quick access to the CambridgeSoft web site from within ChemOffice. With the **Online** menu, you can:

- Register your software.
- Search for compounds by name or ACX number and insert the structure in a worksheet
- Use ACX numbers, or names or structures in the worksheet, to search for chemical information
- Browse the CambridgeSoft website for technical support, documentation, software updates, and more

To use the **Online** menu, you must have internet access.



Registering Online

ChemOffice 2005 applications utilize a new security scheme. In order to activate any ChemOffice application, you must register with the CambridgeSoft website to receive a registration code. Upon filling out a registration form, the registration code is sent to you by email. This registration scheme does not apply to site licenses.

If your serial number is invalid for any reason, or if you do not have an internet connection, you will have to contact CambridgeSoft Support to receive a registration code.

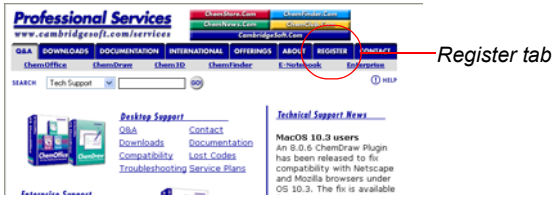
You may use your ChemOffice application a limited number of times while waiting for the registration process to be completed. Once the application times out, you must register to activate the software.

In addition to registering your software, you can request literature, or register for limited free access to ChemFinder.com, ChemACX.com, ChemClub.com, and the email edition of ChemBioNews from the **Register Online** link of the **Online** menu. This link connects you to the Cambridgesoft Professional Services page. From this page you can link to a registration form.

To register online:

1. From the **Online** menu, choose **Register Online**.

   The Cambridgesoft Professional Services page opens in your browser.



2. Select the **Register** tab.

Accessing the Online ChemDraw User's Guide

The **Online** menu link **Browse CS ChemDraw Documentation** opens the Cambridgesoft Desktop Manuals page, where you can access current and previous versions of the ChemOffice User's Guide.

To access the CambridgeSoft Manuals page:

1. From the **Online** menu, choose **Browse CS ChemDraw Documentation**.

   The Desktop Manuals page appears. PDF versions of the CambridgeSoft manuals can be accessed from this page.

   NOTE: *If you do not have a CambridgeSoft User account, you will be directed to a sign-up page first.*

2. Click version of the manual to view.

Accessing CambridgeSoft Technical Support

The **Online** menu link **Browse CS ChemOffice Technical Support** also opens the Cambridgesoft Professional Services page. There are a number of links on this page for Troubleshooting, Downloads, Q&A (the ChemOffice FAQ), Contact, and so forth.

Finding Information on ChemFinder.com

The **Find Information on ChemFinder.com** menu item links your browser to the ChemFinder database record of the compound you have selected.

ChemFinder is the public-access database on the ChemFinder.com website. It contains physical, regulatory, and reference data for organic and inorganic compounds.

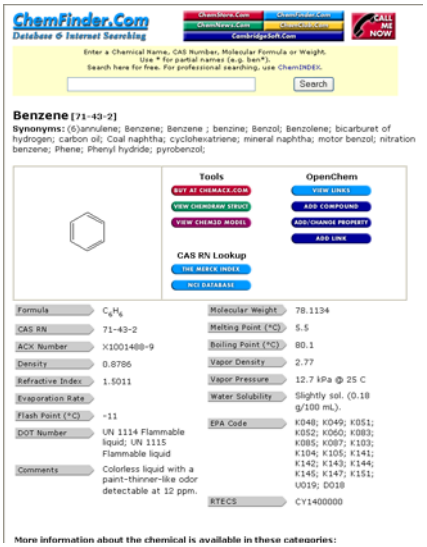
To access ChemFinder.com:

1. In ChemOffice, select a structure you want to look up.
2. From the **Online** menu, choose **Find Information on ChemFinder.com**.

   The ChemFinder.com page opens in your browser with information on the selected structure.

In ChemFinder.com you can search for chemical information by name (including trade names), CAS number, molecular formula, or molecular weight.

Follow the links to do substructure queries.The following illustration shows part of the page for Benzene.



Finding Chemical Suppliers on ACX.com

The **Find Suppliers on ACX.Com** menu item links your browser to the chemacx.com database record of suppliers of the compound you have selected.

ChemACX (Available Chemicals Exchange) is a Webserver application that accesses a database of commercially available chemicals. The database contains catalogs from research and industrial chemical vendors.

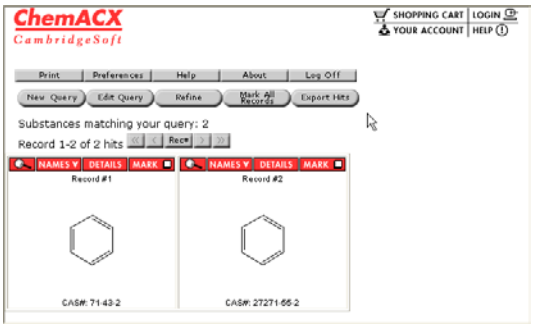
ChemACX allows the user to search for particular chemicals and view a list of vendors providing those chemicals.

To use **Find Suppliers on ACX.Com** menu access:

1. In ChemOffice, select a structure you want to look up.
2. From the **Online** menu, choose **Find Suppliers on ACX.com**.

   The ChemACX.Com page opens in your browser with information on the selected structure.

For example the ChemACX.com page for Benzene is shown below.



For more information on using the ChemACX website, see the ChemOffice Enterprise Workgroup & Databases Manual.

Finding ACX Structures and Numbers

ChemOffice searches ACX and returns information about related structures and numbers. You can place the returned information in your document.

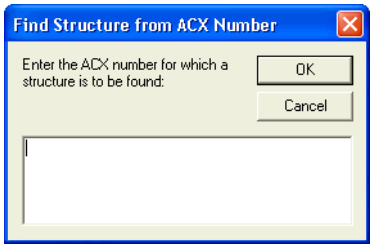
ACX Structures

There are two ways to find ACX structures: by ACX number or by name.

To find a structure that corresponds to an ACX number:

1. From the **Online** menu, choose **Find Structure from ACX Number**.

   The **Find Structure from ACX number** dialog box appears.



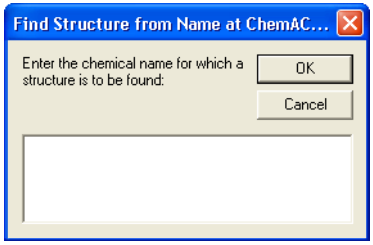
2. Type the ACX registry number.
3. Click **OK**.

   The Structure appears in your document.

To find a structure from a name

1. From the **Online** menu, choose **Find Structure from Name at ChemACX.com**.

   The **Find Structure from Name** dialog box appears.



2. Type in a name. As with ChemFinder.com, you can use a chemical name or a trade name.
3. Click **OK**.

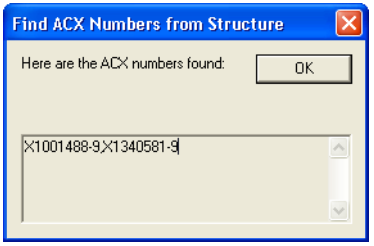
   The Structure appears in your document.

ACX Numbers

To Find an ACX number for a structure:

1. In a ChemOffice document, select the structure for which you want to find an ACX number.
2. From the **Online** menu, choose **Find ACX Numbers from Structure**.

   The ACX number appears in the **Find ACX Numbers from Structure** dialog box.



Browsing SciStore.com

Browse ChemStore.com opens the SciStore (formerly ChemStore) page of the CambridgeSoft web site (http://scistore.cambridgesoft.com/).

To access Browse SciStore.com:

- From the **Online** menu, choose **Browse ChemStore.com**.

  The SciStore.Com page opens in your browser.

You can search SciStore.Com for chemicals, lab supplies, chemistry-related software, and other items you want to buy. You can access ChemACX.Com and other pages from SciStore.Com.

Browsing CambridgeSoft.com

Browse CambridgeSoft.com opens the Home page of the CambridgeSoft web site.

To access the CambridgeSoft Home Page:

- From the **Online** menu, choose **Browse CambridgeSoft.com**.

  The CambridgeSoft web site in your browser.

Check the CambridgeSoft web site for new product information. You can also get to SciStore.Com, ChemBioNews.Com, and other pages through CambridgeSoft.Com.

Using the ChemOffice SDK

The ChemOffice Software Developer's Kit (SDK) enables you to customize your applications.

To browse the ChemOffice SDK:

- From the **Online** menu, choose **Browse ChemOffice SDK**.

  The CS ChemOffice SDK page opens in your browser.

TechnicalSupport
CambridgeSoft.Com/Support
CS ChemOffice Software Developer's Kit
Welcome to the CS ChemOffice software developer's kit (SDK) web site that provides documentation, sample code, and other resources for the ChemOffice component Application Programming Interfaces (APIs). You can use these APIs to create custom add-ons that enhance ChemOffice functionality or to add ChemOffice functionality to your programs. If you cannot find the code or samples on this site you are looking for, we may be able to provide you with what you need. Please contact consulting with the details or your code request.
Unless otherwise indicated, the information present on this site applies to the latest versions of our software.
APIs are available for the following ChemOffice components:
ChemDraw

The ChemOffice SDK page contains documentation, sample code, and other resources for the Application Programming Interfaces (APIs).

NOTE: *You must activate Javascript in your browser in order to use the ChemOffice SDK page.*

Appendix B: Technical Support

Overview

CambridgeSoft Corporation (CS) provides technical support to all registered users of this software through the internet, and through our Technical Support department.

Our Technical Support webpages contain answers to frequently asked questions (FAQs) and general information about our software. You can access our Technical Support page using the following address: http://www.cambridgesoft.com/services/

If you don't find the answers you need on our website, please do the following before contacting Technical Support.

1. Check the ReadMe file for known limitations or conflicts.
2. Check the system requirements for the software at the beginning of this User's Guide.
3. Read the Troubleshooting section of this appendix and follow the possible resolution tactics outlined there.
4. If all your attempts to resolve a problem fail, fill out a copy of the CS Software Problem Report Form at the back of the User's Guide. This form is also available on-line at: http://www.cambridgesoft.com/services/mail
   - Try to reproduce the problem before contacting us. If you can reproduce the problem, please record the exact steps that you took to do so.
   - Record the exact wording of any error messages that appear.
   - Record anything that you have tried to correct the problem.

You can deliver your CS Software Problem Report Form to Technical Support by the following methods:

Internet:
http://www.cambridgesoft.com/services/mail

Email: support@cambridgesoft.com

Fax: 617 588-9360

Mail: CambridgeSoft Corporation
ATTN: Technical Support
100 CambridgePark Drive
Cambridge, MA 02140 USA

Serial Numbers

When contacting Technical Support, you must *always* provide your serial number. This serial number was on the outside of the original application box, and is the number that you entered when you launched your CambridgeSoft application for the first time. If you have thrown away your box and lost your installation instructions, you can find the serial number in the following way:

- Choose **About CS <application name>** from the **Help** menu. The serial number appears at the bottom left of the About box.

For more information on obtaining serial numbers and registration codes see:
http://www.cambridgesoft.com/services/codes.cfm

Troubleshooting

This section describes steps you can take that affect the overall performance of CambridgeSoft Desktop Applications, as well as steps to follow if your computer crashes when using a CS software product.

Performance

Below are some ways you can optimize the performance of CambridgeSoft Desktop Applications:

- In the Performance tab in the System control panel, allocate more processor time to the application.
- Install more physical RAM. The more you have, the less ChemOffice Desktop Applications will have to access your hard disk to use Virtual Memory.
- Increase the Virtual Memory (VM). Virtual memory extends RAM by allowing space on your hard disk to be used as RAM. However, the time for swapping between the application and the hard disk is slower than swapping with physical RAM.

  Change the VM as follows:

  - System control panel, Performance tab.

System Crashes

CambridgeSoft Desktop Applications should never crash, but below are the steps you should go through to try to resolve issues that cause computer crashes while using a CS software product.

1. Restart Windows and try to reproduce the problem. If the problem recurs, continue with the following steps.
2. The most common conflicts concern Video Drivers, Printer Drivers, screen savers, and virus protection. If you do need to contact us, be sure to determine what type and version of drivers you are using.

   Video Driver related problems: If you are having problems with the display of any CambridgeSoft Desktop Application, try switching to the VGA video driver in the display Control Panel (or System Setup, and then retest the problems. If using a different driver helps, your original driver may need to be updated–contact the maker of the driver and obtain the most up-to-date driver. If you still have trouble contact us with the relevant details about the original driver and the resulting problem.

   Printer Driver related problems: Try using a different printer driver. If using a different driver helps, your original driver may need to be updated–contact the maker of the driver and obtain the most up-to-date driver. If you still have trouble contact us with the relevant details about the original driver and the resulting problem.
3. Try reinstalling the software. Before you reinstall, uninstall the software and disable all background applications, including screen savers and virus protection. See the complete uninstall instructions on the CambridgeSoft Technical Support web page.
4. If the problem still occurs, use our contact form at: http://www.cambridgesoft.com/services/mail and provide the details of the problem to Technical Support.

Appendix C: Substructures

Overview

You can define substructures and add them to a substructures table. When you define a substructure, the attachment points (where unselected atoms are bonded to selected atoms) are stored with the substructure.

If a substructure contains more than one attachment point (such as Ala), the atom with the lowest serial number normally becomes the first attachment point. The atom with the second lowest serial number becomes the second attachment point, and so on. However, there are situations where this general rule is not valid.

Attachment point rules

The following rules cover all possible situations for multiple attachment points in substructures; Rule 3 is the normal situation described above:

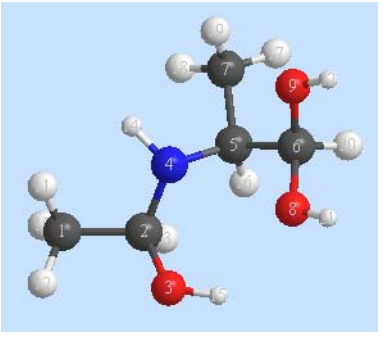
1. If an atom has an open valence and is not attached to an atom that is unselected, it goes after any atom that is attached to an unselected atom.
2. If an atom is attached only to rectification atoms, it goes after any atom that is attached to non-rectification atoms.
3. If two atoms are the same according to the above criteria, the atom with the lowest serial number goes first.
4. If two atoms are the same according to the above criteria, then the one which is attached to the atom with the lowest serial number goes first.

Angles and measurements

In addition to the attachment points, the measurements between the selected atoms and nearby unselected atoms are saved with the substructure to position the substructure relative to other atoms when the substructure is used to convert labels into atoms and bonds.

For example, Chem3D stores with the substructure a dihedral angle formed by two atoms in the substructure and two unselected atoms. If more than one dihedral angle can be composed from selected (substructure) and unselected (non-substructure) atoms, the dihedral angle that is saved with the substructure consists of the atoms with the lowest serial numbers.

Consider the following model to define a substructure for alanine:



Since polypeptides are specified beginning with the N-terminal amino acid, N(4) should have a lower serial number than the Carboxyl C(6). To ensure that a chain of alanine substructures is formed correctly, C(1) should have a lower serial number than O(3) so that the C-C-N-C dihedral angle is used to position adjacent substructures within a label.

Defining Substructures

To define a substructure:

1. Build a model of the substructure. You can use Chem3D tools, or build it in the ChemDraw panel.
2. Select the atoms to define.
3. From the Edit menu, choose Copy.

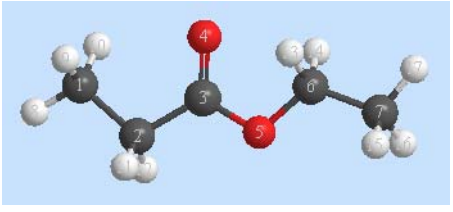
To save the substructure definition:

1. Open Substructures.xml. From the
2. View menu, point to Parameter Tables and choose Substructures.
3. Right-click in the Substructures table and choose Append Row.

   A new row is added to the table.
4. Select the cell in the Model column.
5. Right-click in the cell and choose Paste from the context menu.

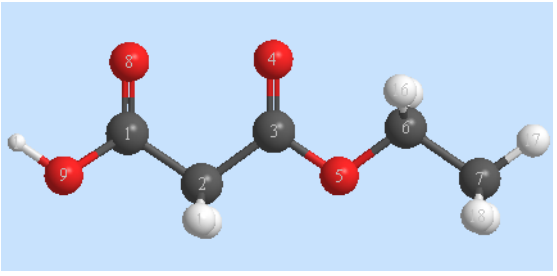
   The structure is pasted into the table cell. Note that it will be not be visible until you move to another cell.
6. Select the cell in the Name column.
7. Type a name for the substructure.
8. Close and save the Substructures table.

For example, consider an ester substructure, R_1COOR_2. You can build this substructure as part of the following model:



Select atoms 3-5 (the two oxygens and the carbon between them) and using the instructions above, create a new record in the Substructures Table.

If you want to append an ester onto the end of the chain as a carboxylic acid, you can simply double-click a hydrogen to replace it with the ester (as long as the name of the substructure is in the text box). Replacing H(8) (of the original structure) would produce the following structure:



Notice that the carbon atom in the ester has replaced the hydrogen. This is because, when the ester was defined, the carbon atom had a lower serial number (3) than the oxygen atom that formed the other attachment point in the substructure (5).

NOTE: *When defining substructures with multiple attachment points, it is critical to note the serial numbers of the atoms in the substructure so that you can correctly orient the substructure when it is inserted in the model. See the rules for multiple attachment points discussed at the beginning of this section.*

Appendix D: Atom Types

Overview

Chem3D assigns atom types when you build with Automatically Correct Atom Types turned on. You can also create your own atom types.

Assigning Atom Types

When you replace atoms, Chem3D attempts to assign the best atom type to each atom by comparing the information about the atom (such as its symbol and the number of bonds to the atom) to each atom type record in the Atom Type table.

When you have selected the Automatically Correct Atom Types check box in the Building control panel, atom types are corrected when you delete atoms or bonds, or when you add atoms or bonds. In addition, if this check box is selected, then the atom types of pre-existing atoms may change when you replace other atoms with other atoms of a different type.

If the wrong atom type is assigned to an atom, you can specify the correct atom type by selecting the Text Building Tool, clicking the atom, typing the name of the atom type into the text box, and pressing the Enter key.

Atom Type Characteristics

The characteristics of an atom must match the following atom type characteristics for Chem3D to assign the atom type to the atom.

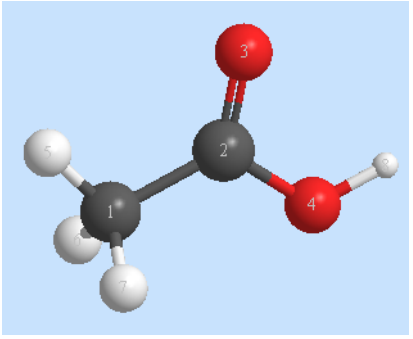
- The symbol.
- The bound-to type (if specified for the atom type).
- The bound-to order (if the bound-to type is specified).
- The number of double, triple and delocalized bonds.

NOTE: *For comparing bond orders, an atom type that contains one double bond may be assigned to an atom that contains two delocalized bonds. For example, all six carbons in benzene are C Alkene.*

If the maximum ring size field of an atom type is specified, then the atom must be in a ring of that size or smaller to be assigned the corresponding atom type.

If an atom is bound to fewer ligands than are specified by an atom type geometry but the rectification type is specified, then the atom can be assigned to that atom type. Chem3D fills the open valences with rectification atoms.

For example, consider the atom types for the following structure:



O(3) matches the criteria specified for the atom type O Carbonyl. Specifically, it is labeled 'O', it is bound to a C Carbonyl by a double bond and it is attached to exactly one double bond and no triple bonds.

If an atom can be assigned to more than one atom type, atom types are assigned to atoms in the following order:

1. Atom types whose bound-to types are specified and are not the same as their rectification types.
2. Atom types whose bound-to types are specified and are the same as their rectification types.
3. Atom types whose bound-to types are not specified.

For example**,** in the model depicted above, O(4) could be one of several atom types. First, it could be an O Ether atom for which the bound-to type is unspecified (priority number 3, above). Alternatively, it could be an O Alcohol for which the bound-to type is the same as the rectification type, H Alcohol (priority number 2, above). A third possibility is O Carboxyl, for which the bound-to type is C Carbonyl and the rectification type is H Carboxyl (priority number 1). Because the characteristic of a specified bound-to type which is not the same as the rectification type (number 1 in the priority list above) is given precedence over the other two possibilities, the O Carboxyl atom type is assigned to the oxygen atom.

Defining Atom Types

If you need to define atom types, whether to add to the atom types table for building or to add to a file format interpreter for importing, here is the general procedure:

To add or edit an atom type to the Atom Types table:

1. From the **View** menu, point to Parameter Tables and choose Atom Types.

   The Atom Types table opens in a window.
2. To edit an atom type, click in the cell that you want to change and type new information.
3. Enter the appropriate data in each field of the table. Be sure that the name for the parameter is not duplicated elsewhere in the table.
4. Close and Save the table.

   You now can use the newly defined atom type.

Appendix E: Keyboard Modifiers

The following tables list the keyboard modifiers that allow you to manipulate your view of the model without changing tools.

Rotation

Key	Drag	Shift+Drag
ALT	Trackball rotate view	Trackball rotate model selection
B		Rotate 1/2 of fragment around bond
V	Rotate view about selected axis	Rotate model selection about axis
X	Rotate view about view X axis	Rotate model about view X axis
Y	Rotate view about view Y axis	Rotate model about view Y axis
Z	Rotate view about view Z axis	Rotate model about view Z axis

In addition to the keyboard shortcuts, you can rotate a model by dragging with the mouse while holding down both the middle mouse button or scroll wheel and the left mouse button. *Tip: The order is important; press the middle button first.*

Zoom and Translate

Key	Drag	Shift+Drag
CTRL	Translate view	Translate model selection
A	Zoom to center	

Key	Drag	Shift+Drag
Q	Zoom to rotation center	
W	Zoom to selection center	

If you have a wheel mouse, you may also use the scroll wheel to zoom. Dragging with the middle button or scroll wheel translates the view.

Selection

Standard Selection

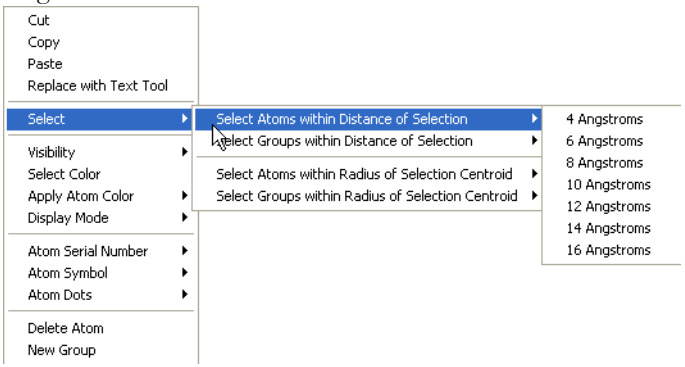
Key	Click	Shift+Click	Drag	Shift+Drag
S	Select atom/bond	Multiple select atom/bond	Box select atoms /bonds	Multiple box select atoms /bonds

Notes:

- Clicking a bond selects the bond and the two atoms connected to it.
- Double-clicking an atom or bond selects the fragment that atom or bond belongs to.
- Double-clicking a selected fragment selects the next higher fragment; that is, each double-click moves you up one in the hierarchy until you have selected the entire model.

Radial Selection

Radial selection is selection of an object or group of objects based on the distance or radius from a selected object or group of objects. This feature is particularly useful for highlighting the binding site of a protein. Radial selection is accessed through the **Select** submenu of the context menu in the Model Explorer or 3D display.



In all cases, multiple selection is specified by holding the shift key down while making the selections.

Submenu option	Effect
Select Atoms within Distance of Selection	Selects all atoms (except for those already selected) lying within the specified distance from any part of the current selection. The current selection will be un-selected unless multiple selection is used.
Select Groups within Distance of Selection	Selects all groups (except for those already selected) that contain one or more atoms lying within the specified distance from any part of the current selection. The current selection will be un-selected unless multiple selection is used.
Select Atoms within Radius of Selection Centroid	Selects all atoms (except for those already selected) lying within the specified distance of the centroid of the current selection. The current selection will be un-selected unless multiple selection is used.
Select Groups within Radius of Selection Centroid	Selects all groups (except for those already selected) that contain one or more atoms lying within the specified distance of the centroid of the current selection. The current selection will be un-selected unless multiple selection is used.

Appendix F: 2D to 3D Conversion

Overview

This section discusses how Chem3D performs the conversion from two to three dimensions when opening a ChemDraw or ISIS/Draw document, when pasting a ChemDraw or ISIS/Draw structure from the Clipboard, or when opening a ChemDraw connection table file. While Chem3D can read in and assimilate any ChemDraw structure, you can assist Chem3D in the two- to three-dimensional conversion of your models by following the suggestions in this Appendix.

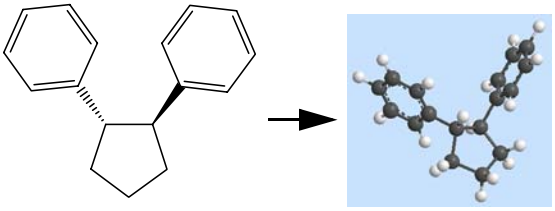
Chem3D uses the atom labels and bonds drawn in ChemDraw to form the structure of your model. For every bond drawn in ChemDraw, a corresponding bond is created in Chem3D. Every atom label is converted into at least one atom.

Dative bonds are converted to single bonds with a positive formal charge added to one atom (the atom at the tail of the dative bond) and a negative formal charge added to the other (the head of the dative bond).

Stereochemical Relationships

Chem3D uses the stereo bonds and H-Dot and H-Dash atom labels in a ChemDraw structure to define the stereochemical relationships in the corresponding model. Wedged bonds in ChemDraw indicate a bond where the atom at the wide end of the bond is in front of the atom at the narrow end of the bond. Wedged hashed bonds indicate the opposite: the atom at the wide end of a wedged hashed bond is behind the atom at the other end of the bond.

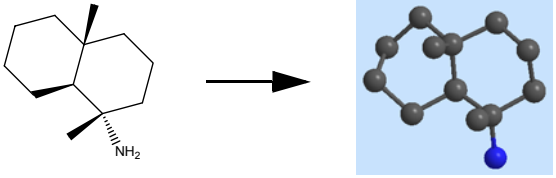
Example 1



In Example 1, the two phenyl rings are trans about the cyclopentane ring. The phenyl ring on the left is attached by a wedged hashed bond; the phenyl ring on the right is attached by a wedged bond.

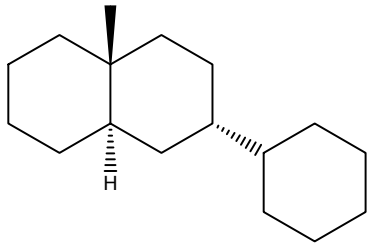
You can also use dashed, hashed, and bold bonds. However, you should be aware of potential ambiguity where these non-directional bonds are used. A dashed, hashed, or bold bond must be between one atom that has at least three attachments and one atom that has no more than two attachments, including the dashed, hashed, or bold bond.

Example 2



In Example 2, the nitrogen atom is placed behind the ring system and the two methyl groups are placed in front of the ring system. Each of these three atoms is bonded to only one other atom, so they are presumed to be at the wide ends of the stereo bonds.

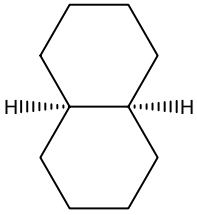
Example 3



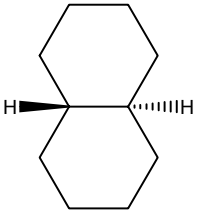
In Example 3, however, the hashed bond is ambiguous because both atoms on the hashed bond are attached to more than two bonds. In this case the hashed bond is treated like a solid bond. Wavy bonds are always treated like solid bonds.

H-Dots and H-Dashes are also used to indicate stereochemistry. H-Dots become hydrogen atoms attached to carbon atoms by a wedged bond. H-Dashes become hydrogen atoms attached by a wedged hashed bond.

Example 4



cis-decalin



trans-decalin

Example 4 shows cis-decalin on the left and trans-decalin on the right as they would be drawn in ChemDraw to be read in by Chem3D. Of course, you can specify a cis fusion with two H-Dots instead of two H-Dashes.

As a general rule, the more stereo bonds you include in your model, the greater is the probability that Chem3D will make correct choices for chirality and dihedral angles.

When converting two-dimensional structures, Chem3D uses standard bond lengths and angles as specified in the current set of parameters. If Chem3D tries to translate strained ring systems, the ring closures will not be of the correct length or angle.

Labels

Chem3D uses the atom labels in a two-dimensional structure to determine the atom types of the atoms. Unlabeled atoms are assumed to be carbon. Labels are converted into atoms and bonds using the same method as that used to convert the text in a text box into atoms and bonds. Therefore, labels can contain several atoms or even substructures.

Appendix G: File Formats

Editing File Format Atom Types

Some file formats contain information describing the atom types that the file format understands. Typically, these atom types are ordered by some set of numbers, similar to the atom type numbers used in the Atom Types table. If the file format needs to support additional types of atoms, you can supply those types by editing the file format atom types.

Chem3D 9.0 uses XML tables for storing file formats. You can edit these tables in any text editor or in Chem3D by selecting the table you want to edit from the Parameter Tables list on the View menu.

> ***TIP:*** *The .xml files are in the path ...\Chem3D\C3D Items*

Name

Each atom type is described by a name. This name is a number found in files of the format described by the file format. All names must be unique. The records in the table window are sorted by name.

> ***NOTE:*** *While names are similar to atom type numbers, they do not have to correspond to the atom type numbers of atom types. In some cases, however, they do correspond.*

Description

The second field contains a description of the atom type, such as C Alkane. This description is included for your reference only.

The remaining fields (Symbol, Charge, Maximum Ring Size, Rectification type, Geometry, Number of Double Bonds, Number of Triple Bonds, Number of Delocalized Bonds, Bound to Order and Bound to Type) contain information corresponding to the information in an Atom Types table.

File Format Examples

The following sections provide examples of the files created when you save Chem3D files using the provided file formats.

Alchemy File

The following is a sample Alchemy file[1] (Alchemy) created using Chem3D for a model of cyclohexanol. The numbers in the first column are line numbers that are added for reference only.

1	19 ATOMS	19 BONDS		
2	1 C3	-1.1236	-0.177	0.059
3	2 C3	-0.26	-0.856	-1.0224
4	3 C3	1.01	-0.0491	-1.3267
5	4 C3	1.838	0.1626	-0.0526
6	5 C3	0.9934	0.8543	1.0252
7	6 C3	-0.2815	0.0527	1.3275
8	7 O3	-2.1621	-1.0585	0.3907
9	8 H	-1.4448	0.8185	-0.3338
10	9 H	-0.8497	-0.979	-1.9623
11	10 H	0.0275	-1.8784	-0.6806
12	11 H	1.6239	-0.5794	-2.0941
13	12 H	0.729	0.9408	-1.7589

1. Alchemy III is a registered trademark of Tripos Associates, Inc.

14	13 H	2.197	-0.8229	0.3289
15	14 H	2.7422	0.7763	-0.282
16	15 H	1.5961	0.9769	1.9574
17	16 H	0.7156	1.8784	0.679
18	17 H	-0.8718	0.6068	2.0941
19	18 H	-0.004	-0.9319	1.7721
20	19 H	-2.7422	-0.593	0.9688
21	1	1	2	SINGLE
22	2	1	6	SINGLE
23	3	1	7	SINGLE
24	4	1	8	SINGLE
25	5	2	3	SINGLE
26	6	2	9	SINGLE
27	7	2	10	SINGLE
28	8	3	4	SINGLE
29	9	3	11	SINGLE
30	10	3	12	SINGLE
31	11	4	5	SINGLE
32	12	4	13	SINGLE
33	13	4	14	SINGLE
34	14	5	6	SINGLE
35	15	5	15	SINGLE
36	16	5	16	SINGLE
37	17	6	17	SINGLE
38	18	6	18	SINGLE
40	19	7	19	SINGLE

Each line represents a data record containing one or more fields of information about the molecule. Each field is delimited by spaces or a tab. The fields used by Chem3D are described below:

1. Line 1 contains two fields. The first field is the total number of atoms in the molecule and the second field is the total number of bonds.
2. Lines 2–20 each contain 5 fields of information about each of the atom in the molecule. The first field is the serial number of the atom. The second field is the atom type, the third field is the X coordinate, the fourth field is the Y coordinate and the fifth field is the Z coordinate.

NOTE: *Atom types in the Alchemy file format are user-definable. See "Editing File Format Atom Types" on page 241 for instructions on modifying or creating an atom type.*

3. Lines 21–40 each contain 4 fields describing information about each of the bonds in the molecule. The first field is the bond number (ranging from 1 to the number of bonds), the second field is the serial number of the atom where the bond begins, the third field is the serial number of the atom where the bond ends, and the fourth field is the bond type. The possible bond types are: SINGLE, DOUBLE, TRIPLE, AMIDE, or AROMATIC. Note that all the bond order names are padded on the right with spaces to eight characters.

FORTRAN Formats

The FORTRAN format for each record of the Alchemy file is as follows:

Line Number	Description	FORTRAN Format
1	number of atoms, number of bonds	I5, 1X, ATOMS,1X,I5, 1X, BONDS
2–20	atom serial number, type, and coordinates	I6,A4,3(F9.4)
21–40	bond id, from atom, to atom, bond type	I6,I5,I6,2X,A8

Cartesian Coordinate Files

The Cartesian coordinate file format (Cart Coords, Cart Coords 2) interprets text files that specify models in terms of the X, Y, and Z coordinates of the atoms. This file format can also interpret fractional cell coordinates in orthogonal or non-orthogonal coordinate systems.

Atom Types in Cartesian Coordinate Files

Two file formats are supplied with Chem3D that interpret Cartesian coordinate files. The difference between the two file formats are the codes used to convert atom type numbers in the file into atom types used by Chem3D.

In Cartesian coordinates 1, atom types are numbered according to the numbering used by N.L. Allinger in MM2. These numbers are also generally followed by the program PC Model.

In Cartesian coordinates 2, the atom type number for all atom types is computed by multiplying the atomic number of the element by 10 and adding the number of valences as specified by the geometry of the atom type. These numbers are also generally followed by the program MacroModel.

For example, the atom type number for C Alkane (a tetrahedral carbon atom) is 64.

To examine the atom types described by a file format, see "Editing File Format Atom Types" on page 241.

The Cartesian Coordinate File Format

The format for Cartesian coordinate files is as follows:

1. The first line of data contains the number of atoms in the model.

   Optionally, you can follow the number of atoms in the file with crystal cell parameters for the crystal structure: a, b, c, α, β, and γ.

   Following the cell parameters, you can also include an exponent. If you include an exponent, then all of the fractional cell coordinates will be divided by 10 raised to the power of the exponent.

2. The first line of a Cartesian coordinate file is followed by one line of data for each atom in the model. Each line describing an atom begins with the symbol for the atom. This symbol must correspond to a symbol in the Elements table. The symbol can include a charge, such as N+. The symbol is followed by the serial number.

3. The serial number is followed by the three coordinates of the atom. If you have specified crystal cell parameters in the first line of the file, then these numbers are the fractional cell coordinates. Otherwise, the three numbers are X, Y, and Z Cartesian coordinates.

4. Following the coordinates is the atom type number of the atom type for this atom. This number must correspond to the code of an atom type record specified in the file format atom type table. For more information, see "Editing File Format Atom Types" on page 241.

5. Following the atom type number is the connection table for the atom. You can specify up to ten other atoms. The connection table for a Cartesian coordinate file can be listed in one of two ways: by serial number or by position.

   Connection tables by serial number use the serial number of each atom to determine the number that appears in the connection table of other atoms. All serial numbers must, therefore, be unique.

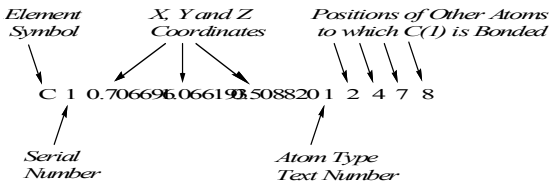
Connection tables by position use the relative positions of the atoms in the file to determine the number for each atom that will appear in the connection table of other atoms. The first atom is number 1, the second is 2, etc.

6. To create multiple views of the same set of atoms, you can flow the descriptions of the atoms with an equal number of lines corresponding to the same atoms with different coordinates. Chem3D generates independent views using the additional sets of coordinates.

Samples of Cartesian coordinate files with connection tables by position and serial number for a model of cyclohexanol are shown below. To clearly illustrate the difference between the two formats, the serial number of the oxygen has been set to 101.

19									
C	1	0.706696	1.066193	0.50882	1	2	4	7	8
C	2	-0.834732	1.075577	0.508789	1	1	3	9	10
C	3	-1.409012	0.275513	-0.668915	1	2	6	11	12
C	4	1.217285	-0.38632	0.508865	1	1	5	13	14
C	5	0.639328	-1.19154	-0.664444	1	4	6	15	16
C	6	-0.89444	-1.1698	-0.646652	1	3	5	17	18
O	101	1.192993	1.809631	1.59346	6	1	19		
H	9	1.052597	1.559525	-0.432266	5	1			
H	10	-1.211624	2.125046	0.457016	5	2			
H	11	-1.208969	0.640518	1.465607	5	2			
H	12	-2.524918	0.2816	-0.625809	5	3			
H	13	-1.11557	0.762314	-1.629425	5	3			
H	14	0.937027	-0.8781	1.470062	5	4			
H	15	2.329758	-0.41023	0.437714	5	4			
H	16	1.003448	-2.24631	-0.618286	5	5			
H	17	1.005798	-0.76137	-1.627	5	5			
H	18	-1.295059	-1.73161	-1.524567	5	6			
H	19	-1.265137	-1.68524	0.271255	5	6			
H	102	2.127594	1.865631	1.48999	21	7			

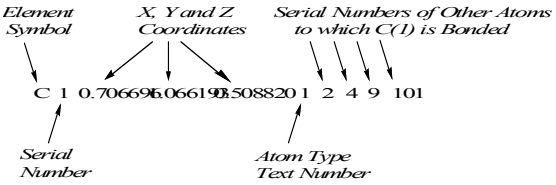
Following is an example of a Cartesian Coordinate file with Connection table by Position for Cyclohexanol.


Element Symbol
X, Y and Z Coordinates
Positions of Other Atoms to which C(1) is Bonded
C 1 0.706696 1.066193 0.50882 1 2 4 7 8
Serial Number
Atom Type
Text Number

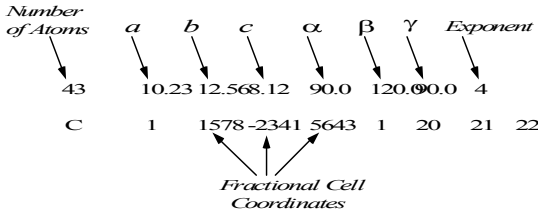
An example of a Cartesian Coordinate File with Connection Table by Serial Number for Cyclohexanol follows.

19									
C	1	0.706696	1.066193	0.50882	1	2	4	9	10
C	2	-0.834732	1.075577	0.508789	1	1	3	10	11
C	3	-1.409012	0.275513	-0.668915	1	2	6	12	13
C	4	1.217285	-0.38632	0.508865	1	1	5	14	15
C	5	0.639328	-1.19154	-0.664444	1	4	6	16	17
C	6	-0.89444	-1.1698	-0.646652	1	3	5	18	19
O	101	1.192993	1.809631	1.59346	6	1	102		
H	9	1.052597	1.559525	-0.432266	5	1			
H	10	-1.211624	2.125046	0.457016	5	3			
H	11	-1.208969	0.640518	1.465607	5	3			
H	12	-2.524918	0.2816	-0.625809	5	4			
H	13	-1.11557	0.762314	-1.629425	5	4			
H	14	0.937027	-0.8781	1.470062	5	5			
H	15	2.329758	-0.41023	0.437714	5	5			
H	16	1.003448	-2.24631	-0.618286	5	6			
H	17	1.005798	-0.76137	-1.627	5	6			
H	18	-1.295059	-1.73161	-1.524567	5	7			
H	19	-1.265137	-1.68524	0.271255	5	7			
H	102	2.127594	1.865631	1.48999	21	10			
						1			

Components of a Cartesian coordinate File with Connection Table by Serial Number for C(1) of Cyclohexanol is shown below.


Element Symbol
X, Y and Z Coordinates
Serial Numbers of Other Atoms to which C(1) is Bonded
C 1 0.706696 1.066193 0.50882 2 4 9 101
Serial Number
Atom Type Text Number

Components of a Cartesian coordinate File with Crystal coordinate Parameters for C(1) is shown below.



FORTRAN Formats

The FORTRAN format for the records in a Cartesian coordinate file with a connection table by serial number or position and a Cartesian coordinate file with fractional crystal cell parameters are listed in the following tables:

Cartesian coordinate File (Connection Table by Serial Number or Position):

Line Number	Description	FORTRAN Format
1	Number of Atoms	I3
2 to End	Atom coordinates	A3, 1X, I4, 3(1X, F11.6), 1X, I4, 10(1X, I4)

Cartesian coordinate File (Fractional Crystal Cell Parameters):

Line Number	Description	FORTRAN Format
1	Number of Atoms, Crystal Cell Parameters	I3, 6(1X, F), I
2 to End	Atom coordinates	A3, 1X, I4, 3(1X, F11.6), 1X, I4, 10(1X,I4)

Cambridge Crystal Data Bank Files

The specific format of Cambridge Crystal Data Bank files (CCDB) used by Chem3D is the FDAT format, described on pages 26–42 of the data file specifications of the Cambridge Structural Database, Version 1 File Specifications from the Cambridge Crystallographic Data Centre. For further details about the FDAT format, please refer to the above publication or contact the Cambridge Crystallographic Data Centre.

As described in the specifications of the Cambridge Crystal Data Bank format, bonds are automatically added between pairs of atoms whose distance is less than that of the sum of the covalent radii of the two atoms. The bond orders are guessed based on the ratio of the actual distance to the sum of the covalent radii. The bond orders, bond angles, and the atom symbols are used to determine the atom types of the atoms in the model.

Bond Type	Actual Distance / Sum of Covalent Radii
Triple	0.81
Double	0.87
Delocalized	0.93
Single	1.00

Internal Coordinates File

Internal coordinates files (INT Coords) are text files that describe a single molecule by the internal coordinates used to position each atom. The serial numbers are determined by the order of the atoms in the file. The first atom has a serial number of 1, the second is number 2, etc.

The format for Internal coordinates files is as follows:

1. Line 1 is a comment line ignored by Chem3D. Each subsequent line begins with the atom type number of an atom type.
2. Line 2 contains the atom type number of the Origin atom.
3. Beginning with line 3, the atom type number is followed by the serial number of the atom to which the new atom is bonded and the distance to that atom. In an Internal coordinates file, the origin atom is always the first distance-defining atom in the file. All distances are measured in Angstroms.
4. Beginning with line 4, the distance is followed by the serial number of the first angle-defining atom and the angle between the newly defined atom, the distance-defining atom, and the first angle-defining atom. All angles are measured in degrees.
5. Beginning with line 5, the serial number of a second angle-defining atom and a second defining angle follows the first angle. Finally, a number is given that indicates the type of the second angle. If the second angle type is zero, the second angle is a dihedral angle: New Atom – Distance-defining Atom – First Angle-defining Atom – Second Angle-defining Atom. Otherwise the third angle is a bond angle: New Atom – Distance-defining Atom – Second Angle-defining Atom. If the second angle type is 1, then the new atom is defined using a Pro-R/Pro-S relationship to the three defining atoms; if the second angle type is -1, the relationship is Pro-S.

NOTE: *You cannot position an atom in terms of a later-positioned atom.*

The following is a sample of an Internal coordinates output file for cyclohexanol which was created from within Chem3D:

```
1
1    1    1.54146
1    2    1.53525    1    111.7729
1    1    1.53967    2    109.7132    3    -55.6959    0
1    4    1.53592    1    111.703     2    55.3112     0
1    3    1.53415    2    110.7535    1    57.0318     0
6    1    1.40195    2    107.6989    3    -172.6532   0
5    1    1.11742    2    109.39      4    109.39      -1
5    2    1.11629    1    109.41      3    109.41      1
5    2    1.11568    1    109.41      3    109.41      -1
5    3    1.11664    2    109.41      6    109.41      -1
5    3    1.11606    2    109.41      6    109.41      1
5    4    1.11542    1    109.41      5    109.41      1
5    4    1.11493    1    109.41      5    109.41      -1
5    5    1.11664    4    109.41      6    109.41      1
5    5    1.11617    4    109.41      6    109.41      -1
5    6    1.11664    3    109.41      5    109.41      1
```

```
5     6     1.11606     3     109.41     5     109.41     -1
21    7     0.942       1     106.8998   2     59.999     0

5     6
```

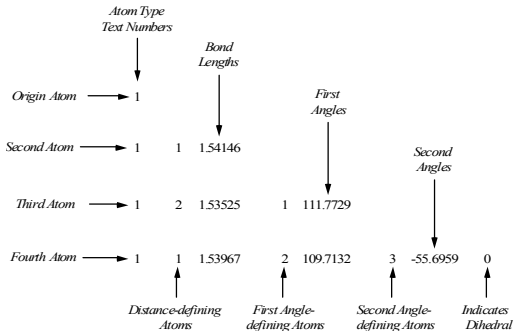
Bonds

Bonds are indicated in Internal coordinates files in two ways.

First, a bond is automatically created between each atom (except the Origin atom) and its distance-defining atom.

Second, if there are any rings in the model, ring-closing bonds are listed at the end of the file. If there are ring-closing bonds in the model, a blank line is included after the last atom definition. For each ring-closure, the serial numbers of the two atoms which comprise the ring-closing bond are listed on one line. The serial number of the first atom is 1, the second is 2, etc. In the prior Internal coordinates output example of cyclohexanol, the numbers 5 and 6 are on a line at the end of the file, and therefore the ring closure is between the fifth atom and the sixth atom.

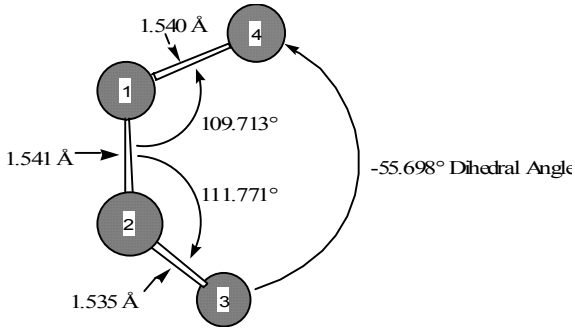
If a bond listed at the end of an Internal coordinates format file already exists (because one of the atoms on the bond is used to position the other atom on the bond) the bond is removed from the model. This is useful if you want to describe multiple fragments in an internal coordinates file.



Components of an Internal coordinates File for C(1) through C(4) of Cyclohexanol

In this illustration, the origin atom is C(1). C(2) is connected to C(1), the origin and distance defining atom, by a bond of length 1.54146 Å. C(3) is connected to C(2) with a bond of length 1.53525 Å, and at a bond angle of 111.7729 degrees with C(1), defined by C(3)-C(2)-C(1). C(4) is attached to C(1) with a bond of length 1.53967 Å, and at a bond angle of 109.7132 degrees with C(2), defined by C(4)-C(1)-C(2). C(4) also forms a dihedral angle of -55.6959 degrees with C(3), defined by C(4)-C(1)-C(2)-C(3).

This portion of the Internal coordinates file for C(1) through C(4) of Cyclohexanol can be represented by the following structural diagram:



FORTRAN Formats

The FORTRAN formats for the records in an Internal coordinates file are as follows:

Line Number	Description	FORTRAN Format
Comment	Ignored by Chem3D	
Origin Atom		I4
Second Atom		I4, 1X, I3, 1X, F9.5
Third Atom		I4, 2(1X, I3, 1X, F9.5)
Fourth Atom to Last Atom		I4, 3(1X, I3, 1X, F9.5), I4
Blank Line		
Ring Closure Atoms		2(1X, I4)

MacroModel

MacroModel is produced within the Department of Chemistry at Columbia University, New York, N.Y. The MacroModel file format is defined in the "MacroModel Structure Files" version 2.0 documentation. The following is a sample MacroModel file created using Chem3D. The following file describes a model of cyclohexanol.

```
19 cyclohexanol
3  2  1  6  1  7  1  18 1  0  0  0  0  -1.396561  0.350174  1.055603  0
3  1  1  3  1  8  1  9  1  0  0  0  0  -0.455032  -0.740891 1.587143  0
3  2  1  4  1  10 1  11 1  0  0  0  0  0.514313   -1.222107 0.49733   0
3  3  1  5  1  12 1  13 1  0  0  0  0  1.302856   -0.04895  -0.103714 0
3  4  1  6  1  14 1  15 1  0  0  0  0  0.372467   1.056656  -0.627853 0
3  1  1  5  1  16 1  17 1  0  0  0  0  -0.606857  1.525177  0.4599    0
41 1  1  0  0  0  0  0  0  0  0  0  0  0  -2.068466  -0.083405 0.277008  0
41 2  1  0  0  0  0  0  0  0  0  0  0  0  -1.053284  -1.603394 1.96843   0
41 2  1  0  0  0  0  0  0  0  0  0  0  0  0.127151   -0.3405   2.451294  0
41 3  1  0  0  0  0  0  0  0  0  0  0  0  1.222366   -1.972153 0.925369  0
41 3  1  0  0  0  0  0  0  0  0  0  0  0  -0.058121  -1.742569 -0.306931 0
```

41	4	1	0	0	0	0	0	0	0	0	0	0	1.972885	0.38063	0.679077	0
41	4	1	0	0	0	0	0	0	0	0	0	0	1.960663	-0.413223	-0.928909	0
41	5	1	0	0	0	0	0	0	0	0	0	0	0.981857	1.921463	-0.992111	0
41	6	1	0	0	0	0	0	0	0	0	0	0	-1.309372	2.283279	0.037933	0
41	6	1	0	0	0	0	0	0	0	0	0	0	-0.033539	2.031708	1.272888	0
41	1	1	0	0	0	0	0	0	0	0	0	0	-2.052933	0.717285	1.881104	0
42	15	1	0	0	0	0	0	0	0	0	0	0	0.275696	0.374954	-2.411163	0

Each line represents a data record containing one or more fields of information about the model. Each field is delimited by space(s) or a tab.

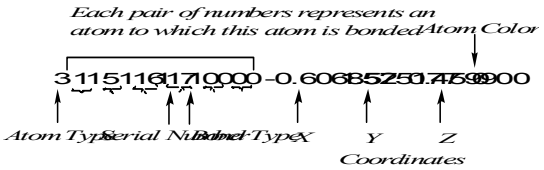
The fields in the MacroModel format file used by Chem3D are:

1. Line 1 contains 2 fields: the first field is the number of atoms and the second field is the name of the molecule. The molecule name is the file name when the file is created using Chem3D.
2. Lines 2-19 each contain 17 fields describing information about one atom and its attached bond. The first field contains the atom type. The second through thirteenth fields represent 6 pairs of numbers describing the bonds that this atom makes to other atoms. The first number of each pair is the serial number of the other atom, and the second number is the bond type. The fourteenth field is the X coordinate, the fifteenth field is the Y coordinate, the sixteenth field is the Z coordinate and finally, and the seventeenth field is the color of the atom.

   Atom colors are ignored by Chem3D. This field will contain a zero if the file was created using Chem3D.

NOTE: *Atom types are user-definable. See "Editing File Format Atom Types" on page 241 for instructions on modifying or creating an atom type.*

For example, the following illustrates the atom and bond components for C6 and bond 3 of cyclohexanol:



FORTRAN Formats

The FORTRAN format for each record of the MacroModel format is as follows:

Line Number	Description	FORTRAN Format
1	number of atoms and molecule name (file name	1X,I5,2X,A

MDL MolFile

The MDL MolFile[1] format is defined in the article "Description of Several Chemical Structure File Formats Used by Computer Programs Developed at Molecular Design Limited" found in the Journal

1. MDL MACCS-II is a product of MDL Information Systems, Inc. (previously called Molecular Design, Limited).

of Chemical Information and Computer Science, Volume 32, Number 3, 1992, pages 244–255. The following is a sample MDL MolFile file created using Chem3D Pro. This file describes a model of cyclohexanol (the line numbers are added for reference only):

1	cyclohexanol								
2									
3									
4	19	19	0	0	0				
5	-1.3488	0.1946	1.0316	C	0	0	0	0	0
6	-0.4072	-0.8965	1.5632	C	0	0	0	0	0
7	0.5621	-1.3777	0.4733	C	0	0	0	0	0
8	1.3507	-0.2045	-0.1277	C	0	0	0	0	0
9	0.4203	0.9011	-0.6518	C	0	0	0	0	0
10	-0.559	1.3696	0.4359	C	0	0	0	0	0
11	-0.3007	0.4266	-1.7567	O	0	0	0	0	0
12	-2.0207	-0.239	0.253	H	0	0	0	0	0
13	-2.0051	0.5617	1.8571	H	0	0	0	0	0
14	-1.0054	-1.7589	1.9444	H	0	0	0	0	0
15	0.1749	-0.4961	2.4273	H	0	0	0	0	0
16	1.27	-2.1277	0.9014	H	0	0	0	0	0
17	-0.0103	-1.8981	-0.3309	H	0	0	0	0	0
18	2.0207	0.225	0.6551	H	0	0	0	0	0
19	2.0084	-0.5688	-0.9529	H	0	0	0	0	0
20	1.0296	7659	-1.0161	H	0	0	0	0	0
21	-1.2615	2.1277	0.0139	H	0	0	0	0	0
22	0.0143	1.8761	1.2488	H	0	0	0	0	0
23	0.3286	0.2227	-2.4273	H	0	0	0	0	0
24	1	2	1	0	0	0			
25	1	6	1	0	0	0			
26	1	8	1	6	0	0			
27	1	9	1	1	0	0			
28	2	3	1	6	0	0			
29	2	10	1	0	0	0			
30	2	11	1	1	0	0			
31	3	4	1	0	0	0			

32	3	12	1	0	0	0
33	3	13	1	6	0	0
34	4	5	1	0	0	0
35	4	14	1	1	0	0
36	4	15	1	6	0	0
37	5	6	1	1	0	0
38	5	7	1	6	0	0
39	5	16	1	0	0	0
40	6	17	1	0	0	0
41	6	18	1	1	0	0
42	7	19	1	6	0	0

Each line represents either a blank line, or a data record containing one or more fields of information about the structure. Each field is delimited by a space(s) or a tab.

The fields in the MDL MolFile format used by Chem3D Pro are discussed below:

1. Line 1 starts the header block, which contains the name of the molecule. The molecule name is the file name when the file was created using Chem3D Pro.
2. Line 2 continues the Header block, and is a blank line.
3. Line 3 continues the Header block, and is another blank line.
4. Line 4 (the Counts line) contains 5 fields which describes the molecule: The first field is the number of atoms, the second field is the number of bonds, the third field is the number of atom lists, the fourth field is an unused field and the fifth field is the stereochemistry.

NOTE: *Chem3D Pro ignores the following fields: number of atom lists, the unused field and stereochemistry. These fields will always contain a zero if the file was created using Chem3D Pro.*

5. Lines 5–23 (the Atom block) each contain 9 fields which describes an atom in the molecule: The first field is the X coordinate, the second field is the Y coordinate, the third field is the Z coordinate, the fourth field is the atomic symbol, the fifth field is the mass difference, the sixth field is the charge, the seventh field is the stereo parity designator, the eighth field is the number of hydrogens and the ninth field is the center.

NOTE: *Chem3D Pro ignores the following fields: mass difference, charge, stereo parity designator, number of hydrogens, and center. These fields contain zeros if the file was created using Chem3D Pro.*

6. Lines 24–42 (the Bond block) each contain 6 fields which describe a bond in the molecule: the first field is the from-atom id, the second field is the to-atom id, the third field is the bond type, the fourth field is the bond stereo designator, the fifth field is an unused field and the sixth field is the topology code.

NOTE: *Chem3D Pro ignores the unused field and topology code. These fields will contain zeros if the file was created using Chem3D Pro.*

Limitations

The MDL MolFile format does not support non-integral charges in the same way as Chem3D Pro. For example, in a typical MDL MolFile format file, the two oxygens in a nitro functional group (NO_2) contain different charges: -1 and 0. In Chem3D models, the oxygen atoms each contain a charge of -0.500.

FORTRAN Formats

The FORTRAN format for each record of the MDL MolFile format is as follows:

Line Number	Description	FORTRAN Format
1	Molecule name (file name)	A
2	Blank line	
3	Blank line	
4	Number of atoms Number of bonds	5I3
5–23	Atom coordinates, atomic symbol	3F10.4,1X,A2,5I3
24–42	Bond id, from atom, to atom, and bond type	6(1X,I2)

MSI MolFile

The MSI MolFile is defined in Chapter 4, "Chem-Note File Format" in the Centrum: Chem-Note™ Application documentation, pages 4-1 to 4-5. The following is a sample MSI MolFile file created using Chem3D Pro for cyclohexanol (the line numbers are added for purposes of discussion only):

```
 1    ! Polygen 133
 2    Polygen Corporation: ChemNote molecule file (2D)
 3    * File format version number
 4    90.0928
 5    * File update version number
 6    92.0114
 7    * molecule name
 8    cyclohexanol-MSI
 9    empirical formula
10    Undefined Empirical Formula
11    * need 3D conversion?
12    0
```

```
13      * 3D displacement vector
14      0.000 0.000 0.000
15      * 3D rotation matrix
16      1.000 0.000 0.000 0.000 1.000 0.000 0.000 0.000 1.000
17      * 3D scale factor
18      0
19      * 2D scale factor
20      1
21      * 2D attributes
22      1 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23      * 3D attributes
24      0 0 0 0 0 0 0 0 0 0 0 0
25      * Global display attributes
26      1 0 1 12 256
27      * Atom List
28      * Atom# Lbl Type x y x y z bits chrg ichrg frag istp lp chrl ring frad name seg grp FLAGS
29      1       C       10      0       0       -1      0.46    0.2     0       0       0 0 0 0 0 0 0 C 1 0 -1 0 0 0 0 0 0 [C]
30      2       C       10      0       0       1.2     -1.1    0.2     0       0       0 0 0 0 0 0 0 C 2 0 -1 0 0 0 0 0 0 [C]
30      2       C       10      0       0       1.2     -1.1    0.2     0       0       0 0 0 0 0 0 0 C 2 0 -1 0 0 0 0 0 0 [C]
31      3       C       10      0       0       0.1     -1.6    0.7     0       0       0 0 0 0 0 0 0 C 3 0 -1 0 0 0 0 0 0 [C]
32      4       C       10      0       0       1.3     -1.1    0       0       0       0000000C40-1000000[C]
33      5       C       10      0       0       1.2     0.48    0       0       0       0 0 0 0 0 0 0 C 5 0 -1 0 0 0 0 0 0 [C]
34      6       C       10      0       0       0       1.01    -1      0       0       0 0 0 0 0 0 0 C 6 0 -1 0 0 0 0 0 0 [C]
35      7       O       45      0       0       0       2.42    -1      0       0       0 0 0 0 0 0 0 O 7 0 -1 0 0 0 0 0 0 [O]
36      8       H       8       0       0       0.6     2.72    -1      0       0       0 0 0 0 0 0 0 H 7 0 -1 0 0 0 0 0 0 [H]
37      9       H       1       0       0       2.1     0.86    -1      0       0       0 0 0 0 0 0 0 H 8 0 -1 0 0 0 0 0 0 [H]
38      10      H       1       0       0       1.4     0.86    0.8     0       0       0 0 0 0 0 0 0 H 9 0 -1 0 0 0 0 0 0 [H]
39      11      H       1       0       0       1.1     -1.4    -1      0       0       0 0 0 0 0 0 0 H 10 0 -1 0 0 00 00[H]
40      12      H       1       0       0       2.2     -1.4    0.2     0       0       0 0 0 0 0 0 0 H 11 0 -1 0 0 0000 [H]
41      13      H       1       0       0       0       0.72    -2      0       0       0 0 0 0 0 0 0 H 12 0 -1 0 0000 0 [H]
42      14      H       1       0       0       0.1     -2.7    0.7     0       0       0 0 0 0 0 0 0 H 13 0 -1 0 0 0000 [H]
43      15      H       1       0       0       0.3     -1.3    1.7     0       0       0 0 0 0 0 0 0 H 14 0 -1 0 0 0 00 [H]
44      16      H       1       0       0       -1      -1.5    -1      0       0       0 0 0 0 0 0 0 H 15 0 -1 0 0 0000 [H]
45      17      H       1       0       0       -2      -1.5    0.9     0       0       0 0 0 0 0 0 0 H 16 0 -1 0 0 0000 [H]
46      18      H       1       0       0       -1      0.85    1.2     0       0       0 0 0 0 0 0 0 H 17 0 -1 0 0 0000 [H]
47      19      H       1       0       0       -2      0.83    0       0       0       0 0 0 0 0 0 0 H 18 0 -1 0 0 0000 [H]
```

```
48      * Bond List
49      * Bond# bond_type atom1 atom2 cis/trans length locked ring Sh_type Sh_nr Qorder Qtopol Qs
50      1 1 1 2 0                       0.000 0 0 0 0 [S] 0 0
51      2 1 1 6 0                       0.000 0 0 0 0 [S] 0 0
52      3 1 1 18 0                      0.000 0 0 0 0 [S] 0 0
53      4 1 1 19 0                      0.000 0 0 0 0 [S] 0 0
54      5 1 2 3 0                       0.000 0 0 0 0 [S] 0 0
55      6 1 2 16 0                      0.000 0 0 0 0 [S] 0 0
56      7 1 2 17 0                      0.000 0 0 0 0 [S] 0 0
57      8 1 3 4 0                       0.000 0 0 0 0 [S] 0 0
58      9 1 3 14 0                      0.000 0 0 0 0 [S] 0 0
59      10 1 3 15 0                     0.000 0 0 0 0 [S] 0 0
60      11 1 4 5 0                      0.000 0 0 0 0 [S] 0 0
61      12 1 4 11 0                     0.000 0 0 0 0 [S] 0 0
62      13 1 4 12 0                     0.000 0 0 0 0 [S] 0 0
63      14 1 5 6 0                      0.000 0 0 0 0 [S] 0 0
64      15 1 5 9 0                      0.000 0 0 0 0 [S] 0 0
65      16 1 5 10 0                     0.000 0 0 0 0 [S] 0 0
66      17 1 6 7 0                      0.000 0 0 0 0 [S] 0 0
67      18 1 6 13 0                     0.000 0 0 0 0 [S] 0 0
68      19 1 7 8 0                      0.000 0 0 0 0 [S] 0 0
69      * Bond Angles
70      * bond1 bond2 angle locked
71      * Dihedral Angles
72      * at1-cons at1 at2 at2-cons angle locked
73      * Planarity data
74      * User data area
75      * End of File
```

The MSI MolFile[1] format is broken up into several sections. Section headers are preceded by a "*". Blank lines also contain a "*". Each line is either a blank line, a header line or a data record containing one or more fields of information about the structure. Individual fields are delimited by space(s) or a tab. The fields in the MSI MolFile format file used by Chem3D Pro are discussed below.

1. Molecular Simulations MOLFILE (ChemNote) is a product of Molecular Simulations, Inc.

The field value for Carbon 6 from the example file is included in parentheses for reference:

1. Line 1 is a standard header line for MSI MolFile format files.
2. Line 2 normally indicates the application which created the file.
3. Line 3 is the header for the File format version number section.
4. Line 4 indicates the file format version number. The format for this field is YY.MMDD.
5. Line 5 is the header for the File update version number section.
6. Line 6 indicates the file update version number. The format for this field is YY.MMDD.
7. Line 7 is the header for the molecule name section.
8. Line 8 contains the field molecule name. This field contains either the file name, or "Undefined Name".
9. Line 9 is the header for the empirical formula.
10. Line 10 contains the empirical formula field. This field contains either the empirical formula or "Undefined Empirical Formula".
11. Lines 11–24 each contains information concerning conversions from 3D to 2D.
12. Line 25 is the header for the Global display attributes section.
13. Line 26 contains 5 fields describing the global display attributes: Line thickness (1), font style (0), type face (1), type size (12), font (256). These values are specific to the platform that is generating the file.
14. .Line 27 contains the header for the Atom Lists section.
15. Line 28 contains a listing of all the possible fields for the atom list section. When the file is created using Chem3D Pro the following fields are used: Atom#,Lbl, Type, and x,y,z.
16. Lines 29–47 each contains 28 fields describing information about each of the atoms in the structure: the first field is the atom number (6), the second field is the atom label (C), the third field is the atom type (10), the fourth field and fifth fields contain 2D coordinates, and contain zeros when the file is created using Chem3D Pro, the sixth field is the X coordinate (-0.113) and the fifth field is the Y coordinate (1.005), the sixth field is the Z coordinate (-0.675), the seventh through fifteenth fields are ignored and contain zeros when the file is created by Chem3D Pro, the sixteenth field is, again, the atom label (C), the eighteenth field is, again, the atom number (6), the nineteenth field is the segment field, the twentieth field is the coordination field, the twenty first field is ignored, the twenty-second field is called the saturation field: if the atom is attached to any single, double or delocalized bonds this field is 1 (not saturated) otherwise this field is 0. The twenty-third through the twenty-sixth fields are ignored and contain zeros when the file is created using Chem3D Pro, the twenty-seventh field is, again, the atom label (C).

NOTE: *Atom types in the Molecular Simulations MolFile format are user-definable. For more information, see "Editing File Format Atom Types" on page 241.*

---

17. Line 48 contains the header for the Bond List section.
18. Line 49 contains a listing of all the possible fields for the bond list section. When the file is created by Chem3D Pro the following fields are used: Bond#, Bond_type, atom 1, atom 2 and cis/trans and Qorder.
19. Lines 50–68 each contain 4 fields describing information about each of the bonds in the structure: the first field is the internal bond number (6), the second field is the bond type (1), the third and fourth fields are the atom

serial numbers for the atoms involved in the bond [atom 1 (2), atom 2 (16)], the fifth field is the cis/trans designator (this is 0 if it does not apply), the sixth through tenth fields are ignored, and contain zeros if the file is created using Chem3D Pro, the eleventh field contains the bond order ([S] meaning single), the twelfth and thirteenth fields are ignored and contain zeros if the file is created using Chem3D Pro.

20. Lines 69–73 are each a section header for 3D conversion use. This section only contains the header name only (as shown) when the file is created using Chem3D Pro.
21. Line 74 is a header for the section User data area. This section contains the header name only (as shown) when the file is created using Chem3D Pro.
22. Line 75 is a header that indicates the End of File.

FORTRAN Formats

The FORTRAN format for each record of the Molecular Simulations MolFile format is as follows:

Line Number	Description	FORTRAN Format
29-47	atom list, field value	I,1X,A,3(1X,I),3F9.3,1X,I,F4.1,7(1X,I),1X,A,I,8(1X,I),“[“,A, “] “
50-68	bond list, field values	I,4(1X,I),F9.3,4(2X,I),1X, “[“,A1, “] “,2(1X,I)

MOPAC

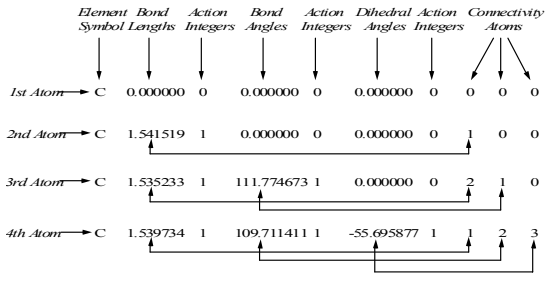
The specific format of the MOPAC files used by Chem3D is the MOPAC Data-File format. This format is described on pages 1-5 through 1-7 of the “Description of MOPAC” section and page 3-5 of the “Geometry Specification” section in the MOPAC Manual (fifth edition). For further details about the MOPAC Data-File format, please refer to the above publication.

The following is a sample MOPAC output file from Chem3D for cyclohexanol:

```
Line 1:
Line 2:  Cyclohexanol
Line 3:
Line 4a: C  0          0  0          0  0          0  0  0  0
Line 4b: C  1.54152    1  0          0  0          0  1  0  0
Line 4c: C  1.53523    1  111.7747    1  0          0  2  1  0
Line 4d: C  1.53973    1  109.7114    1  -55.6959   1  1  2  3
```

Line 4e:	C	1.53597	1	111.7012	1	55.3112	1	4	1	2
Line 4f:	C	1.53424	1	110.7535	1	57.03175	1	3	2	1
Line 4g:	O	1.40196	1	107.6989	1	-172.662	1	1	2	3
Line 4h:	H	1.11739	1	107.8685	1	62.06751	1	1	2	3
Line 4I:	H	1.11633	1	110.0751	1	-177.17	1	2	1	4
Line 4j:	H	1.11566	1	109.4526	1	65.43868	1	2	1	4
Line 4k:	H	1.11665	1	109.9597	1	178.6209	1	3	2	1
Line 4l:	H	1.1161	1	109.5453	1	-63.9507	1	3	2	1
Line 4m:	H	1.11542	1	109.4316	1	-66.0209	1	4	1	2
Line 4n:	H	1.11499	1	110.549	1	176.0838	1	4	1	2
Line 4o:	H	1.11671	1	109.93	1	-178.296	1	5	4	1
Line 4p:	H	1.11615	1	109.4596	1	64.43501	1	5	4	1
Line 4q:	H	1.11664	1	110.0104	1	-178.325	1	6	3	2
Line 4r:	H	1.11604	1	109.6082	1	64.09581	1	6	3	2
Line 4s:	H	0.94199	1	106.898	1	-173.033	1	7	1	2

The following illustrates the components of the MOPAC Output File from Chem3D for C(1) Through C(4) of Cyclohexanol


Element Symbol
Bond Lengths
Action Integers
Bond Angles
Action Integers
Dihedral Angles
Action Integers
Connectivity Atoms
1st Atom C 0.000000 0 0.000000 0 0.000000 0 0 0 0
2nd Atom C 1.541519 1 0.000000 0 0.000000 0 1 0 0
3rd Atom C 1.535233 1 111.774673 1 0.000000 0 2 1 0
4th Atom C 1.539734 1 109.711411 1 -55.695877 1 1 2 3

The internal coordinates section of the MOPAC Data-File format contains one line of text for each atom in the model. Each line contains bond lengths, bond angles, dihedral angles, action integers, and connectivity atoms.

As shown in the illustration above, C(1) is the origin atom. C(2) is connected to C(1) with a bond of length 1.541519 Å. C(3) is connected to C(2) with a bond of length 1.535233 Å, and is at a bond angle of 111.774673 degrees from C(1). C(4) is connected to C(1) with a bond of length 1.539734 Å, and is at a bond angle of 109.711411 degrees from C(2). C(4) also forms a dihedral angle of -55.695877 degrees with C(3).

The action integers listed next to each measurement are instructions to MOPAC which are as follows:

1Optimize this internal coordinate

0Do not optimize this internal coordinate

-1Reaction coordinate or grid index

When you create a MOPAC file from within Chem3D, an action integer of 1 is automatically assigned to each non-zero bond length, bond angle, and dihedral angle for each atom record in the file.

FORTRAN Formats

The description of the MOPAC Data-File format for each line is as follows:

Line Number	Description	Read by Chem3D	Written by Chem3D
1	Keywords for Calculation Instructions	No	No
2	Molecule Title	No	Yes
3	Comment	No	No
4a-s	Internal coordinates for molecule	Yes	Yes
5	Blank line, terminates geometry definition	Yes	Yes

The FORTRAN format for each line containing internal coordinate data in the MOPAC Data-File is FORMAT(1X, 2A, 3(F12.6, I3), 1X, 3I4).

Protein Data Bank Files

The Protein Data Bank file format (Protein DB) is taken from pages 3, 14–15, and 17–18 of the Protein Data Bank Atomic coordinate and Bibliographic Entry Format Description dated January, 1985.

A Protein Data Bank file can contain as many as 32 different record types. Only the COMPND, ATOM, HETATM, and CONECT records are used by Chem3D; all other records in a Protein Data Bank file are ignored. The COMPND record contains the name of the molecule and identifying information.

The ATOM record contains atomic coordinate records for "standard" groups, and the HETATM record contains atomic coordinate records for "non-standard" groups. The CONECT record contains the atomic connectivity records.

NOTE: *The COMPND record is created by Chem3D to include the title of a Chem3D model only when you are saving a file using the Protein Data Bank file format. This record is not used when opening a file.*

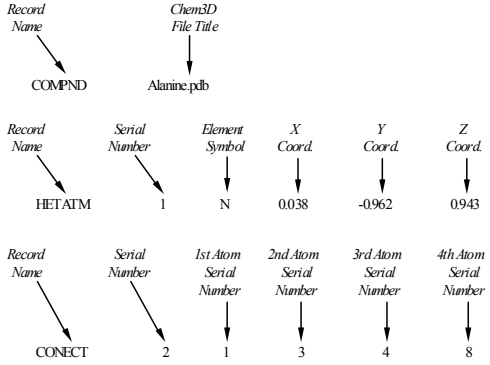
The following is an example of a Protein Data Bank Output File from Chem3D for L-Alanine.

```
COMPND  Alanine.pdb
HETATM  1   N   0   -0.962  1
HETATM  2   C   0   -0.049  0
HETATM  3   C   0.6 0.834   -1
HETATM  4   C   -2  0.834   1
HETATM  5   O   0.3 1.737   -1
HETATM  6   O   1.8 0.459   0
HETATM  7   H   0.9 -1.398  1
HETATM  13  H   -1  -1.737  1
HETATM  8   H   -1  -0.642  -1
HETATM  9   H   -2  1.564   0
HETATM  10  H   -1  1.41    1
HETATM  11  H   -2  0.211   1
HETATM  12  H   2.4 1.06    -1
CONECT  1   2   7   13
CONECT  2   1   3   4   8
CONECT  3   2   5   6
```

```
CONECT    4    2    9   10   11
CONECT    5    3
CONECT    6    3   12
CONECT    7    1
CONECT   13    1
CONECT    8    2
CONECT    9    4
CONECT   10    4
CONECT   11    4
CONECT   12    6
END
```

The ATOM or HETATM record contains the record name, followed by the serial number of the atom being described, the element symbol for that atom, then the X, Y, and Z Cartesian coordinates for that atom.

A CONECT record is used to describe the atomic connectivity. The CONECT records contain the record name, followed by the serial number of the atom whose connectivity is being described, then the serial numbers of the first atom, second atom, third atom and fourth atom to which the described atom is connected.



FORTRAN Formats

The full description of the COMPND record format in Protein Data Bank files is as follows:

Column Number	Column Description	Used by Chem3D
1-6	Record Name (COMPND)	Yes
7-10	UNUSED	No
11-70	Name of Molecule	Yes

The full description of the ATOM and HETATM record formats in Protein Data Bank files is as follows:

Column Number	Column Description	Used by Chem3D
1-6	Record Name (HETATM or ATOM)	Yes
7-11	Atom Serial Number	Yes
12	UNUSED	No
13–16	Atom Name (Element Symbol)	Yes
17	Alternate Location Indicator	No
18–20	Residue Name	Optional

21	UNUSED	No
22	Chain Identifier	No
23–26	Residue Sequence Number	No
27	Code for insertions of residues	No
28–30	UNUSED	No
31–38	X Orthogonal Å coordinates	Yes
39–46	Y Orthogonal Å coordinates	Yes
47–54	Z Orthogonal Å coordinates	Yes
55–60	Occupancy	No
61–66	Temperature Factor	No
67	UNUSED	No
68–70	Footnote Number	No

The full description of the CONECT record format in Protein Data Bank files is as follows:

Column Number	Column Description	Used by Chem3D
1–6	Record Name (CONECT)	Yes
7–11	Atom Serial Number	Yes
12–16	Serial Number of First Bonded Atom	Yes
17–21	Serial Number of Second Bonded Atom	Yes
22–26	Serial Number of Third Bonded Atom	Yes
27–31	Serial Number of Fourth Bonded Atom	Yes
32–36	Hydrogen Bonds, Atoms in cols. 7–11 are Donors	No
37–41	Hydrogen Bonds	No
42–46	Salt Bridge, Atoms in cols. 7–11 have Negative Charge	No
47–51	Hydrogen Bonds, Atoms in cols 7–11 are Acceptors	No
52–56	Hydrogen Bonds	No
57–61	Salt Bridge, Atoms in cols. 7–11 have Positive Charge	No

The FORTRAN formats for the records used in the Protein Data Bank file format are as follows:

Line Description	FORTRAN Format

COMPND	'COMPND', 4X, 60A1
ATOM	'ATOM', 2X, I5,1X,A4, 1X, A3,10X, 3F8.3,16X
HETATM	'HETATM', I5,1X,A4,14X,3F8.3,16X
CONECT	'CONECT', 5I5, 30X

ROSDAL

The Rosdal Structure Language[1] file format is defined in Appendix C: Rosdal Syntax, pages 91–108, of the MOLKICK User's Manual. The Rosdal format is primarily used for query searching in the Beilstein Online Database. Rosdal format files are for export only. The following is a sample Rosdal format file created using Chem3D Pro for cyclohexanol:

1-2-3-4-5-6,1-6,2-7H,3-8H,4-9H,5-10H,6-11H,1-12O-13H,1-14H,2-15H, 3-16H,4-17H,5-18H,6-19H.@

1. Rosdal is a product of Softron, Inc.

SMD

The Standard Molecular Data [2]SMD file) file format is defined in the SMD File Format version 4.3 documentation, dated 04-Feb-1987. The following is a sample SMD file produced using Chem3D Pro for cyclohexanol (the line numbers are added for purposes of discussion only).

2. SMD format - H. Bebak AV-IM-AM Bayer AG.

Line 1	>STRT Cyclohexane			
Line 2 DTCR *Chem3D* 00000 05-MAY-92 12:32:26				
Line 3	>CT Cyclohexan 00039			
Line 4	19 19 (A2,5I2) (6I3)			
Line 5	C	0	0	0
Line 6	C	0	0	0
Line 7	C	0	0	0
Line 8	C	0	0	0
Line 9	C	0	0	0
Line 10	C	0	0	0
Line 11	H	0	0	0
Line 12	H	0	0	0
Line 13	H	0	0	0
Line 14	H	0	0	0
Line 15	H	0	0	0
Line 16	O	0	0	0
Line 17	H	0	0	0
Line 18	H	0	0	0
Line 19	H	0	0	0

Line 20	H	0	0	0
Line 21	H	0	0	0
Line 22	H	0	0	0
Line 23	H	0	0	0
Line 24	1	2	1	
Line 25	1	6	1	
Line 26	1	12	1	
Line 27	1	14	1	
Line 28	2	3	1	
Line 29	2	7	1	
Line 30	2	15	1	
Line 31	3	4	1	
Line 32	3	8	1	
Line 33	3	16	1	
Line 34	4	5	1	
Line 35	4	9	1	
Line 36	4	17	1	
Line 37	5	6	1	
Line 38	5	10	1	
Line 39	5	18	1	
Line 40	6	11	1	
Line 41	6	19	1	
Line 42	12	13	1	
Line 43	>CO ANGSTROEM 0020			
Line 44	4	(3I10)		
Line 45	-6903	13566	-4583	
Line 46	-14061	808	125	
Line 47	-4424	-8880	7132	
Line 48	7577	-12182	-1855	
Line 49	14874	594	-6240	
Line 50	5270	10234	-13349	
Line 51	-18551	-4300	-8725	
Line 52	-9815	-18274	9852	
Line 53	4047	-17718	-10879	
Line 54	19321	5600	2685	
Line 55	10636	19608	-16168	

Line 56	-2794	21139	6600
Line 57	2876	15736	11820
Line 58	-14029	20018	-10310
Line 59	-22477	3450	6965
Line 60	-806	-4365	16672
Line 61	14642	-18918	3566
Line 62	23341	-2014	-13035
Line 63	1740	5536	-22837

Each line is either a blank line, a block header line or a data record containing multiple fields of information about the structure. The SMD file is broken down into several blocks of information. The header for each block starts with a > sign. Individual fields are delimited by space(s) or a tab.

The fields in the SMD format file used by Chem3D Pro are discussed below:

1. Line 1 starts the block named STRT. This block contains the molecule name. The molecule name is the file name when the file was created using Chem3D Pro.
2. Line 2 starts the block named DTCR. The information in this line includes the name of the application that created the file and the date and time when the file was generated.
3. Line 3 starts the block named CT which contains the connection table of the compound(s). Also on this line is a 10 character description of the connection table. This will be the same as the file name when the file is generated using Chem3D Pro. Finally, the number of records contained within the CT block is indicated, 39 in the above example.
4. Line 4 of the CT Block contains four fields. The first field is the number of atoms, the second field is the number of bonds, the third field is the FORTRAN format for the number of atoms, and the fourth field is the FORTRAN format for the number of bonds.
5. Lines 5–23 of the CT Block each contain 4 fields describing an atom. The first field is the element symbol (first letter uppercase, second lowercase). The second field is the total number of hydrogens attached to the atom, the third field is the stereo information about the atom and the fourth field is the formal charge of the atom.

   NOTE: *If the file is created using Chem3D Pro, the number of hydrogens, the stereo information and the formal charge fields are not used, and will always contain zeros.*

6. Lines 24–42 of the CT Block each contains 3 fields describing a bond between the two atoms. The first field is the serial number of the atom from which the bond starts, the second field is the serial number of atom where the bond ends, and the third field is the bond order.
7. Line 43 starts the block named CO, The information in this block includes the Cartesian coordinates of all the atoms from the CT block and indicates the type of coordinates used, Angstroms in this example. Also in this line is the number of lines in the block, 20 in this example.
8. Line 44 contains two fields. The first field contains the exponent used to convert the coordinates in the lines following to the

coordinate type specified in line 43. The second field is the FORTRAN format of the atom coordinates.

9. Lines 45–65 each contains three fields describing the Cartesian coordinates of an atom indicated in the CT block. The first field is the X coordinate, the second field is the Y coordinate and the third field is the Z coordinate.

SYBYL MOL File

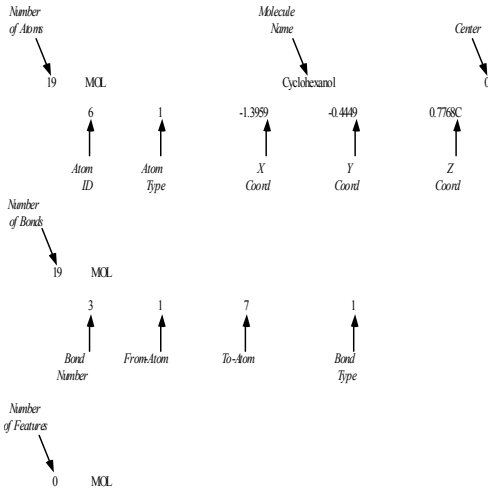
The SYBYL MOL File format (SYBYL) is defined in Chapter 9, "SYBYL File Formats", pages 9–1 through 9–5, of the *1989 SYBYL Programming Manual*.

The following is an example of a file in SYBYL format produced from within Chem3D. This file describes a model of cyclohexanol.

```
19    MOL     Cyclohexanol0
      1    1     1.068     0.3581    -0.7007C
      2    1     -0.207    1.2238    -0.7007C
      3    1     -1.473    0.3737    -0.5185C
      4    1     1.1286    -0.477    0.5913C
      5    1     -0.139    -1.324    0.7800C
      6    1     -1.396    -0.445    0.7768C
      7    8     2.1708    1.2238    -0.7007O
      8    13    1.0068    -0.343    -1.5689H
      9    13    -0.284    1.7936    -1.6577H
      10   13    -0.147    1.9741    0.1228H
      11   13    -2.375    1.032     -0.4983H
      12   13    -1.589    -0.314    -1.3895H
      13   13    1.2546    0.202     1.4669H
      14   13    2.0091    -1.161    0.5742H
      15   13    -0.077    -1.893    1.7389H
      16   13    -0.21     -2.076    -0.0419H
      17   13    -2.308    -1.081    0.8816H
      18   13    -1.372    0.2442    1.6545H
      19   13    2.9386    0.6891    -0.8100H
19    MOL
      1    1     2         1
      2    1     4         1
      3    1     7         1
      4    1     8         1
      5    2     3         1
      6    2     9         1
```

	7	2	10	1
	8	3	6	1
	9	3	11	1
	10	3	12	1
	11	4	5	1
	12	4	13	1
	13	4	14	1
	14	5	6	1
	15	5	15	1
	16	5	16	1
	17	6	17	1
	18	6	18	1
	19	7	19	1
0	MOL			

The following illustration shows the components of the SYBYL Output File from Chem3D for C(6) and Bond 3 of Cyclohexanol.



The format for SYBYL MOL files is as follows:

1. The first record in the SYBYL MOL File contains the number of atoms in the model, the word "MOL", the name of the molecule, and the center of the molecule.
2. The atom records (lines 2–20 in the cyclohexanol example) contain the Atom ID in column 1, followed by the Atom Type in column 2, and the X, Y and Z Cartesian coordinates of that atom in columns 3–5.
3. The first record after the last atom records contains the number of bonds in the molecule, followed by the word "MOL".
4. The bond records (lines 22–40 in the cyclohexanol example) contain the Bond Number in column 1, followed by the Atom ID of the atom where the bond starts (the "From-Atom") in column 2 and the Atom ID of the atom where the bond stops (the "To-Atom") in column 3. The last column in the bond records is the bond type. Finally the last line in the file is the Number of Features

record, which contains the number of feature records in the molecule. Chem3D does not use this information.

FORTRAN Formats

The FORTRAN format for each record of the SYBYL MOL File format is as follows:

Line Description	FORTRAN Format
Number of Atoms/File Name	I4,1X,'MOL',20A2,11X,I4
Atom records	2I4,3F9.4,2A2
Number of Bonds record	I4,1X,'MOL'
Bond records	3I4,9X,I4
Number of Features record	I4,1X,'MOL'

SYBYL MOL2 File

The SYBYL MOL2[1] file format (SYBYL2) is defined in Chapter 3, "File Formats", pages 3033–3050, of the *1991 SYBYL Programming Manual*. The following is a sample SYBYL MOL2 file created using Chem3D Pro. This file describes a model of cyclohexanol (the line numbers are added for reference only):

1. SYBYL is a product of TRIPOS Associates, Inc., a subsidiary of Evans & Sutherland.

```
Line 1    # Name: CYCLOHEXANOL
Line 2
Line 3    @<TRIPOS>MOLECULE
Line 4    CYCLOHEXANOL
Line 5    19 19 0 0 0
Line 6    SMALL
Line 7    NO_CHARGES
Line 8
Line 9
Line 10   @<TRIPOS>ATOM
Line 11   1    C    -1.349   0.195   1.032   C.3
Line 12   2    C    -0.407   -0.896  1.563   C.3
Line 13   3    C    0.562    -1.378  0.473   C.3
Line 14   4    C    1.351    -0.205  -0.128  C.3
Line 15   5    C    0.42     0.9     -0.652  C.3
```

Line 16	6	C	-0.559	1.37	0.436	C.3
Line 17	7	H	-2.021	-0.239	0.253	H
Line 18	8	H	-1.005	-1.759	1.944	H
Line 19	9	H	0.175	-0.496	2.427	H
Line 20	10	H	1.27	-2.128	0.9	H
Line 21	11	H	-0.01	-1.898	-0.331	H
Line 22	12	H	2.021	0.225	0.655	H
Line 23	13	H	2.008	-0.569	-0.953	H
Line 24	14	H	1.03	1.766	-1.016	H
Line 25	15	O	-0.3	0.427	-1.757	O.sp
Line 26	16	H	-1.262	2.128	0.014	H
Line 27	17	H	0.014	1.876	1.249	H
Line 28	18	H	-2.005	0.562	1.857	H
Line 29	19	H	0.329	0.223	-2.427	H.sp
Line 30	@<TRIPOS>BOND					
Line 31	1	31	2	1		
Line 32	2	1	6	1		
Line 33	3	1	7	1		
Line 34	4	1	18	1		
Line 35	5	2	3	1		
Line 36	6	2	8	1		
Line 37	7	2	9	1		
Line 38	8	3	4	1		
Line 39	9	3	10	1		
Line 40	10	3	11	1		
Line 41	11	4	5	1		
Line 42	12	4	12	1		
Line 43	13	4	13	1		
Line 44	14	5	6	1		
Line 45	15	5	14	1		
Line 46	16	5	15	1		
Line 47	17	6	16	1		
Line 48	18	6	17	1		
Line 49	19	15	19	1		

Each line is either a blank line, a section header or a data record containing multiple fields of information about the compound. The SYBYL MOL2 file is broken down into several sections of information. Record type indicators (RTI) break the information about the molecule into sections. RTI's are always preceded by an "@" sign. Individual fields are delimited by space(s) or a tab.

The fields in the SYBYL MOL2 format file used by Chem3D Pro are as follows:

1. Line 1 is a comment field. The pound sign preceding the text indicates a comment line. Name: is a field designating the name of molecule. The molecule name is the file name when the file is created using Chem3D Pro.
2. Line 2 is a blank line.
3. Line 3, "@<TRIPOS>MOLECULE", is a Record Type Indicator (RTI) which begins a section containing information about the molecule(s) contained in the file.

   NOTE: *There are many additional RTIs in the SYBYL MOL2 format. Chem3D Pro uses only @<TRIPOS>MOLECULE, @<TRIPOS>ATOM and @<TRIPOS>BOND.*

4. Line 4 contains the name of the molecule. The name on line 4 is the same as the name on line 1.
5. Line 5 contains 5 fields describing information about the molecule: The first field is the number of atoms, the second field is the number of bonds, the third field is the number of substructures, the fourth field is the number of features and the fifth field is the number of sets.

   NOTE: *Chem3D Pro ignores the following fields: number of substructures, number of features and number of sets. These fields will contain zeros if the file was created using Chem3D Pro.*

6. Line 6 describes the molecule type. This field contains SMALL if the file is created using Chem3D Pro.
7. Line 7 describes the charge type associated with the molecule. This field contains NO_CHARGES if the file is created using Chem3D Pro.
8. Line 8, blank in the above example, might contain internal SYBYL status bits associated with the molecule.
9. Line 9, blank in the above example, might contain comments associated with the molecule.

   NOTE: *Four asterisks appear in line 8 when there are no status bits associated with the molecule but there is a comment in Line 9.*

10. Line 10, "@<TRIPOS>ATOM", is a Record Type Indicator (RTI) which begins a section containing information about each of the atoms associated with the molecule.
11. Lines 11–29 each contain 6 fields describing information about an atom: the first field is the atom id, the second field is the atom name, the third field is the X coordinate, the fourth field is the Y coordinate, the fifth field is the Z coordinate and the sixth field is the atom type.

    NOTE: *Atom types are user-definable See "Editing File Format Atom Types" on page 241 for instructions on modifying or creating an atom type.*

12. Line 30, "@<TRIPOS>BOND", is a Record Type Indicator (RTI) which begins a section containing information about the bonds associated with the molecule.
13. .Lines 31–49 each contain 4 fields describing information about a bond: the first field is the bond id, the second field is the from-atom id, the third field is the to-atom id, and the fourth field is the bond type.

FORTRAN Formats

The FORTRAN format for each record of the SYBYL MOL2 File format is as follows:

Line Number	Description	FORTRAN Format
1	Molecule name (file name)	"# ",5X, "Name: ",1X,A
5	Number of atoms/number of bonds	4(1X,I2)
11–29	Atom type, name, coordinates and id	I4,6X,A2,3X,3 F9.3,2X,A5
31–49	Bond id, from-atom, to-atom, bond type	3I4,3X,A2

Appendix H: Parameter Tables

Parameter Table Overview

Chem3D uses the parameter tables, containing information about elements, bond types, atom types, and other parameters, for building and for analyzing your model.

The parameter tables must be located in the C3D Items directory in the same directory as the Chem3D application.

Parameter Table Use

Chem3D uses several parameter tables to calculate bond lengths and bond angles in your model. To apply this information, select Apply Standard measurements in the Building Control panel.

Calculating the MM2 force field of a model requires special parameters for the atoms and bonds in your model. The MM2 force field is calculated during Energy Minimization, Molecular Dynamics, and Steric Energy computations.

The use of the parameter tables are described in the following table:

Parameter Table	Use
3-Membered Ring Angles.xml	Bond angles for bonds in 3-membered rings. In force field analysis, angle bending portion of the force field for bonds in 3-membered rings.
4-Membered Ring Angles.xml	Bond angles for bonds in 4-membered rings. In force field analysis, angle bending portion of the force field for bonds in 4-membered rings.
4-Membered Ring Torsionals.xml	Computes the portion of the force field for the torsional angles in your model for atoms in 4-membered rings.
Angle Bending Parameters.xml	Standard bond angles. In force field analysis, angle bending portion of the force field for bonds.
Atom Types.xml	Contains atom types available for building models.
Bond Stretching Parameters.xml	Standard bond lengths. In force field analysis, bond stretching and electrostatic portions of force field for bonds.
Conjugated Pisystem Atoms.xml	Bond lengths for bonds involved in Pi systems. Pi system portion of the force field for pi atoms.

Parameter Table	Use
Conjugated Pisystem Bonds.xml	Pi system portion of the force field for pi bonds.
Electronegativity Adjustments.xml	Adjusts optimal bond length between two atoms when one atom is attached to an atom that is electronegative.
Elements.xml	Contains elements available for building models.
MM2 Atom Type Parameters.xml	van der Waals parameters for computing force field for each atom.
MM2 Constants.xml	Constants used for computing MM2 force field.
Out-of-Plane Bending Parameters.xml	Parameters to assure atoms in trigonal planar geometry remain planar. In force field analysis, parameters to assure atoms in trigonal planar geometry remain planar.
References.xml	Contains information about where parameter information is derived.
Substructures.xml	Contains predrawn substructures available for speeding up model building.
Torsional Parameters.xml	Computes the portion of the force field for the torsional angles in your model.
VDW Interactions.xml	Adjusts specific VDW interactions, such as hydrogen bonding.

Parameter Table Fields

Most of the tables contain the following types of fields:

- Atom Type Numbers
- Quality
- Reference

Atom Type Numbers

The first column in a parameter table references an atom type using an Atom Type number. An Atom Type number is assigned to an atom type in the Atom Types table. For example, in Chem3D, a dihedral type field, 1–1–1–4, in the Torsional Parameters table indicates a torsional angle between carbon atoms of type alkane (Atom Type number 1) and carbon atoms of type alkyne (Atom Type number 4). In the 3-membered ring table, the angle type field, 22-22-22, indicates an angle between three cyclopropyl carbons (Atom Type number 22) in a cyclopropane ring.

Quality

The quality of a parameter indicates the relative accuracy of the data.

Quality	Accuracy Level
1	Parameter guessed by Chem3D.
2	Parameter theorized but not confirmed.
3	Parameter derived from experimental data.
4	Parameter well confirmed.

Reference

The reference for a measurement corresponds to a reference number in the References table. References indicate where the parameter data was derived.

Estimating Parameters

In certain circumstances Chem3D may estimate parameters.

For example, during an MM2 analysis, a non-MM2 atom type is encountered in your model. Although the atom type is defined in the Atom Types table, the necessary MM2 parameter will not be defined for that atom type. For example, torsional parameters are missing. This commonly occurs for inorganic complexes, which MM2 does not cover adequately. More parameters exist for organic compounds.

In this case, Chem3D makes an educated "guess" wherever possible. A message indicating an error in your model may appear before you start the analysis. If you choose to ignore this, you can determine the parameters guessed after the analysis is complete.

To view the parameters used in an MM2 analysis:

- From the Calculations menu, point to MM2, and choose Show Used Parameters.

  Estimated parameters have a Quality value of 1.

Creating Parameters

The MM2 force field parameters are based on a limited number of MM2 atom types. These atom types cover the common atom types found in organic compounds. As discussed in the previous section, parameters may be missing from structures containing other than an MM2 atom type.

NOTE: *Adding or changing parameter tables is not recommended unless you are sure of the information your are adding. For example, new parameter information that is documented in journals.*

NOTE: *A method for guessing at missing MM2 Parameters can be found in "Development of an Internal Searching Algorithm for Parameterization of the MM2/MM3 Force Fields", Journal of Computational Chemistry, Vol 12, No. 7, 844–849 (1991).*

To add a new parameter to a parameter table:

1. From the View menu, point to Parameter Tables and choose the parameter table to open.

   The parameter table appears.
2. Right click on a row header and choose Append Row from the context menu.

   A blank row is inserted.

3. Type the information for the new parameter.
4. Close and Save the file.

   The new parameter is added to the file.

NOTE: *Do not include duplicate parameters. If duplicate parameters exist in a parameter table it is indeterminate which parameter will be used when called for in a calculation.*

NOTE: *If you do want to make changes to any of the parameters used in Chem3D, we strongly recommend that you make a back up copy of the original parameter table and remove it from the C3DTABLE directory.*

The Elements

The Elements table (Elements.xml) contains the elements for use in building your models.

To use an element in a model, type its symbol in the Replacement text box (or paste it, after copying the cell in the "Symbol" field to the Clipboard) and press the Enter key when an atom is selected, or double-click an atom. If no atom is selected, a fragment is added.

Four fields comprise a record in the Elements table: the symbol, the covalent radius, the color, and the atomic number.

Symbol

Normally you use only the first column of the Elements table while building models. If you are not currently editing a text cell, you can quickly move from one element to another by typing the first letter or letters of the element symbol.

Covalent Radius

The covalent radius is used to approximate bond lengths between atoms.

Color

The colors of elements are used when the Color by Element check box is selected in the control panel.

To change the color of an element:

- Double-click the current color.

  The Color Picker dialog box appears in which you can specify a new color for the element.

Atom Types

The Atom Types table Atom Types.xml) contains the atom types for use in building your models.

Normally you use only the first column of the Atom Types table while building models. To use an atom type in a model, type its name in the Replacement text box (or paste it, after copying the name cell to the Clipboard) and press the Enter key when an atom is selected, or when you double-click an atom. If no atom is selected, a fragment is added.

Twelve fields comprise an atom type record: name, symbol, van der Waals radius, text number, charge, the maximum ring size, rectification type, geometry, number of double bonds, number of triple bonds, number of delocalized bonds, bound-to order and bound-to type.

Name

The records in the Atom Types table are ordered alphabetically by atom type name. Atom type names must be unique.

Symbol

This field contains the element symbol associated with the atom type. The symbol links the Atom Type table and the Elements table. The element symbol is used in atom labels and when you save files in file formats that do not support atom types, such as MDL MolFile.

van der Waals Radius

The van der Waals (VDW) radius is used to specify the size of atom balls and dot surfaces when displaying the Ball & Stick, Cylindrical Bonds or Space Filling models.

The Close Contacts command in the Measurements submenu of the Structure menu determines close contacts by comparing the distance between pairs of non-bonded atoms to the sum of their van der Waals radii.

The van der Waals radii specified in the Atom Types table do not affect the results of an MM2 computation. The radii used in MM2 computations are specified in the MM2 Atom Types table.

NOTE: *The space filling model display is set in the Model Display tab of the Model Settings dialog box. The appearance of VDW dot surfaces is specified for the entire model in the Atom Display tab of the Model Settings dialog box, or for individual atoms using the Right-click Atom Dots submenu in the Model Explorer.*

Text Number (Atom Type)

Text numbers are used to determine which measurements apply to a given group of atoms in other parameter tables.

For example, C Alkane has an atom type number of 1and O Alcohol has an atom type number of 6. To determine the standard bond length of a bond between a C Alkane atom and an O Alcohol atom , you should look at the 1-6 record in the Bond Stretching table.

Charge

The charge of an atom type is used when assigning atom types to atoms in a model.

When the information about an atom is displayed, the atom symbol is always followed by the charge. Charges can be fractional. For example, the charge of a carbon atom in a cyclopentadienyl ring should be 0.200.

Maximum Ring Size

The maximum ring size field indicates whether the corresponding atom type should be restricted to atoms found in rings of a certain size. If this cell is zero or empty, then this atom type is not restricted. For example, the maximum ring size of C Cyclopropane is 3.

Rectification Type

Possible rectification types are:

- D
- H
- H Alcohol
- H Amide
- H Amine
- H Ammonium
- H Carboxyl
- H Enol
- H Guanidine
- H Thiol

NOTE: *When you specify a rectification type, the bound-to type of the rectification type should not conflict with the atom type. If there is no rectification type for an atom, it is never rectified.*
For example, if the rectification type of O Carboxyl is H Carboxyl, the bound-to type of H Carboxyl should be either O Carboxyl or empty. Otherwise, when assigning atom types, hydrogen atoms bound to O Carboxyl atoms are not assigned H Carboxyl.

Geometry

The geometry for an atom type describes both the number of bonds that extend from this type of atom and the angles formed by those bonds.

Possible geometries are:

- 0 Ligand
- 1 Ligand
- 5 Ligands
- Bent
- Linear
- Octahedral
- Square planar
- Tetrahedral
- Trigonal bipyramidal
- Trigonal planar
- Trigonal pyramidal

NOTE: *Standard bond angle parameters are used only when the central atom has a tetrahedral, trigonal or bent geometry.*

Number of Double Bonds, Triple Bonds, and Delocalized Bonds

The number of double bonds, number of triple bonds, and number of delocalized bonds are integers ranging from zero to the number of ligands as specified by the geometry. Chem3D uses this information both to assign atom types based on the bond orders and to assign bond orders based on atom types.

Bound-to Order

Specifies the order of the bond acceptable between this atom type and the atom type specified in the bound-to type.

For example, for C Carbonyl, only double bonds can be formed to bound-to type O Carboxylate. If there is no bound-to type specified, this field is not used.

Possible bond orders are:

- Single
- Double
- Triple
- Delocalized

NOTE: *The bound-to order should be consistent with the number of double, triple, and delocalized bonds for this atom type. If the bound-to type of an atom type is not specified, its bound-to order is ignored.*

Bound-to Type

Specifies the atom type that this atom must be bound to. If there is no restriction, this field is empty. Used conjunction with the Bound-to Order field.

Non-blank Bound-to-Type values:

- C Alkene
- C Carbocation
- C Carbonyl
- C Carboxylate
- C Cyclopentadienyl
- C Cyclopropene
- C Epoxy
- C Isonitrile
- C Metal CO
- C Thiocarbonyl
- H Alcohol
- H Thiol
- N Ammonium
- N Azide Center
- N Azide End

- N Isonitrile
- N Nitro
- O Carbonyl
- O Carboxylate
- O Epoxy
- O Metal CO
- O Nitro
- O Oxo
- O Phosphate
- P Phosphate
- S Thiocarbonyl

Substructures

The Substructure table (Substructures.xml) contains substructures to use in your model.

To use a substructure simply type its name in the Replacement text box (or paste it, after copying the name cell to the Clipboard) and press the Enter key when an atom(s) is selected, or double-click an atom. You can also copy the substructures picture to the Clipboard and paste it into a model window. The substructure is attached to selected atom(s) in the model window. If no atom is selected, a fragment is added. You can also define your own substructures and add them to the table. The table below shows the substructure table window with the substructure records open (triangles facing down). Clicking a triangle closes the record. The picture of the substructure is minimized.

References

The References table (References.xml) contains information concerning the source for other parameters. Use of the References table does not affect the other tables in any way.

Two fields are used for each reference record: the reference number and the reference description.

Reference Number

The reference number is an index by which the references are organized. Each measurement also contains a reference field that should contain a reference number, indicating the source for that measurement.

Reference Description

The reference description contains whatever text you need to describe the reference. Journal references or bibliographic data are common examples of how you can describe your references.

Bond Stretching Parameters

The Bond Stretching Parameters table (Bond Stretching Parameters.xml) contains information about standard bond lengths between atoms of various atom types. In addition to standard bond lengths are information used in MM2 calculations in Chem3D.

The Bond Stretching table contains parameters needed to compute the bond stretching and electrostatic portions of the force field for the bonds in your model.

The Bond Stretching Parameters record consists of six fields: Bond Type, KS, Length, Bond Dpl, Quality, and Reference.

Bond Type

The Bond Type field contains the atom type numbers of the two bonded atoms.

For example, Bond Type 1-2 is a bond between an alkane carbon and an alkene carbon.

KS

The KS, or bond stretching force constant field, contains a proportionality constant which directly impacts the strength of a bond between two atoms. The larger the value of KS for a particular bond between two atoms, the more difficult it is to compress or to stretch that bond.

Length

The third field, Length, contains the bond length for a particular bond type. The larger the number in the Length field, the longer is that type of bond.

Bond Dipole

The Bond Dpl field contains the bond dipole for a particular bond type. The numbers in this cell give an indication of the polarity of the particular bond. A value of zero indicates that there is no difference in the electronegativity of the atoms in a particular bond. A positive bond dipole indicates that the atom type represented by the first atom type number in the Bond Type field is less electronegative than the atom type represented by the second atom type number. Finally, a negative bond dipole means that the atom type represented by the first atom type number in the Bond Type field is more electronegative than the atom type represented by the second atom type number.

For example, the 1-1 bond type has a bond dipole of zero since both alkane carbons in the bond are of the same electronegativity. The 1-6 bond type has a bond dipole of 0.440 since an ether or alcohol oxygen is more electronegative than an alkane carbon.

Finally, the 1-19 bond type has a bond dipole of - 0.600 since a silane silicon is less electronegative than an alkane carbon.

NOTE: *The 1-5 bond type has a dipole of zero, despite the fact that the carbon and hydrogen atoms on this bond have unequal electronegativity. This approximation drastically reduces the number of dipoles to be computed and has been found to produce acceptable results.*

Record Order

The order of the records in the Bond Stretching table window is as follows:

1. Records are sorted by the first atom type number in the Bond Type field. For example, the record for bond type 1-3 is before the record for bond type 2-3.
2. For records where the first atom type number is the same, the records are sorted by the second atom type number in the Bond Type field. For example, bond type 1-1 is before the record for bond type 1-2.

Angle Bending, 4-Membered Ring Angle Bending, 3-Membered Ring Angle Bending

The Angle Bending table (Angle Bending Parameters.xml) contains information about bond angles between atoms of various atom type. In addition to standard bond angles are information used in MM2 Calculations in Chem3D. Angle bending parameters are used when the central atom has four or fewer attachments and the bond angle is not in a three or four membered ring. In three and

four membered rings, the parameters in the 3-Membered Ring Angles.xml and 4-Membered Ring Angles.xml are used.

The Angle Bending table contains the parameters used to determine the bond angles in your model. In Chem3D Pro, additional information is used to compute the angle bending portions of the MM2 force field for the bond angles in your model.

The 4-membered Ring Angles table contains the parameters that are needed to determine the bond angles in your model that are part of 4-membered rings. In Chem3D, additional information is used to compute the angle bending portions of the MM2 force field for any bond angles in your model which occur in 4-membered rings.

The 3-membered Ring Angles table contains the parameters that are needed to determine the bond angles in your model that are part of 3-membered rings. In Chem3D, additional information is used to compute the angle bending portions of the MM2 force field for any bond angles in your model which occur in 3-membered rings.

Each of the records in the Angle Bending table, the 4-Membered Ring Angles table and the 3-Membered Ring Angles table consists of seven fields: Angle Type, KB, –XR2–, –XRH–, –XH2–, Quality, and Reference.

Angle Type

The first field, Angle Type, contains the atom type numbers of the three atoms which describe the bond angle.

For example, angle type 1-2-1 is a bond angle formed by an alkane carbon bonded to an alkene carbon which is bonded to another alkane carbon. Notice that the alkene carbon is the central atom of the bond angle.

KB

The KB, or the angle bending constant, contains a measure of the amount of energy required to deform a particular bond angle. The larger the value of KB for a particular bond angle described by three atoms, the more difficult it is to compress or stretch that bond angle.

–XR2–

–XR2–, the third field, contains the optimal value of a bond angle where the central atom of that bond angle is not bonded to any hydrogen atoms. In the –XR2– notation, X represents the central atom of a bond angle and R represents any non-hydrogen atom bonded to X.

For example, the optimal value of the 1-1-3 angle type for 2,2-dichloropropionic acid is the –XR2– bond angle of 107.8°, since the central carbon (C-2) has no attached hydrogen atoms.

The optimal value of the 1-8-1 angle type for N,N,N-triethylamine is the –XR2– bond angle of 107.7°, because the central nitrogen has no attached hydrogen atoms. Notice that the central nitrogen has a trigonal pyramidal geometry, thus one of the attached non-hydrogen atoms is a lone pair, the other non-hydrogen atom is a carbon.

–XRH–

The –XRH– field contains the optimal value of a bond angle where the central atom of that bond angle is also bonded to one hydrogen atom and one non-hydrogen atom. In the –XRH– notation, X and R are the same as –XR2–, and H represents a hydrogen atom bonded to X.

For example, the optimal value of the 1-1-3 angle type for 2-chloropropionic acid is the –XRH– bond angle of 109.9°, since the central carbon (C-2) has one attached hydrogen atom. The optimal value of the 1-8-1 angle type for N,N-diethylamine is the –XRH– value of 107.7°, because the central N has

one attached hydrogen atom. In this case the –XR2– and –XRH– values for the 1-8-1 angle type are identical. As in the N,N,N-triethylamine example above, the only attached non-hydrogen atom is a lone pair.

–XH2–

–XH2– is the optimal value of a bond angle where the central atom of that bond angle is also bonded to two hydrogen atoms.

For example, the optimal value of the 1-1-3 angle type for propionic acid is the –XH2– bond angle of 110.0°, since the central carbon (C-2) has two attached hydrogen atoms.

Record Order

When sorted by angle type, the order of the records in the Angle Bending table, the 4-Membered Ring Angles table and the 3-Membered Ring Angles table is as follows:

1. Records are sorted by the second atom type number in the Angle Type field. For example, the record for bond angle type 1-2-1 is before the record for bond angle type 1-3-1.
2. For multiple records where the second atom type number is the same, the records are sorted by the first atom type number in the Angle Type field. For example, the record for bond angle type 1-3-2 is listed before the record for bond angle type 2-3-2.
3. For multiple records where the first two atom type numbers are the same, the records are sorted by the third atom type number in the Angle Type field. For example, the record for bond angle type 1-1-1 is listed before the record for bond angle type 1-1-2.

Pi Atoms

The Pi Atoms table (Conjugated Pisystem Atoms.xml) contains the parameters which are used to correct bond lengths and angles for pi atoms in your model. In Chem3D, additional information is used to compute the pi system portions of the MM2 force field for the pi atoms in your model.

The records in the Pi Atoms table are comprised of six fields: Atom Type, Electron, Ionization, Repulsion, Quality, and Reference.

Atom Type

The Atom type number field contains the atom type number to which the rest of the Conjugated Pisystem Atoms record applies.

Electron

The Electron field contains the number of electrons that a particular pi atom contributes to the pi system.

For example, an alkene carbon, atom type number 2, contributes 1 electron to the pi system whereas a pyrrole nitrogen, atom type number 40, contributes 2 electrons to the pi system.

Ionization

The Ionization field contains the amount of energy required to remove a pi electron from an isolated pi atom. The units of the ionization energy by electron volts (eV). The magnitude of the ionization energy is larger the more electronegative the atom.

For example, an alkene carbon has an ionization energy of -11.160 eV, and the more electronegative pyrrole nitrogen has an ionization energy of -13.145 eV.

Repulsion

The Repulsion field contains a measure of:

- The energy required to keep two electrons, each on separate pi atoms, from moving apart and
- The energy required to keep two electrons, occupying the same orbital on the same pi atom, from moving apart.

  The units of the repulsion energy are electron volts (eV). The repulsion energy is more positive the more electronegative the atom.

For example, an alkene carbon has an repulsion energy of 11.134 eV, and the more electronegative pyrrole nitrogen has an repulsion energy of 17.210 eV.

Pi Bonds

The Pi Bonds table (Conjugated PI System Bonds.xml) contains parameters used to correct bond lengths and bond angles for bonds that are part of a pi system. In Chem3D, additional information is used to compute the pi system portions of the MM2 force field for the pi bonds in a model.

There are five fields in records in the Pi Bonds table: Bond Type, dForce, dLength, Quality, and Reference.

Bond Type

The Bond Type field is described by the atom type numbers of the two bonded atoms.

For example, bond type 2-2 is a bond between two alkene carbons.

dForce

The dForce field contains a constant used to decrease the bond stretching force constant of a particular conjugated double bond. The force constant Kx for a bond with a calculated pi bond order x is:

$K_x = K_2 - (1 - x) * dForce$

where K_2 is the force constant for a non-conjugated double bond, taken from the Bond Stretching table.

The higher the value of K_x for the bond between two pi atoms, the more difficult it is to compress or stretch that bond.

dLength

The dLength field contains a constant used to increase the bond length of any conjugated double bond. The bond length lx for a bond with a calculated pi bond order x is:

$l_x = l_2 + (1 - x) * dLength$

where l_2 is the bond length of a non-conjugated double bond, taken from the Bond Stretching table. The higher the value of l_x for the bond between two pi atoms, the longer that bond is.

Record Order

When sorted for Bond Type, the order of the records in the Conjugated Pisystem Bonds table is as follows:

1. Records are sorted by the first atom type number in the Bond Type field. For example, the record for bond type 2-2 is listed before the record for bond type 3-4.
2. For records where the first atom type number is the same, the records are sorted by the second atom type number in the Bond Type field. For example, the record for bond type 2-2 is listed before the record for bond type 2-3.

Electronegativity Adjustments

The parameters contained in the Electronegativity Adjustments table (Electronegativity Adjustments.xml) are used to adjust the optimal

bond length between two atoms when one of the atoms is attached to a third atom which is electronegative.

For example, the carbon-carbon single bond length in ethane is different than that in ethanol. The MM2 parameter set has only a single parameter for carbon-carbon single bond lengths (1.523Å). The use of electronegativity correction parameters allows the C-C bond in ethanol to be corrected. The electronegativity parameter used in the Electronegativity Corrections table is the 1-1-6 angle type, where atom type 1 is a C Alkane and atom type 6 is an O Alcohol. The value of this parameter is -0.009Å. Thus the C-C bond length in ethanol is 0.009Å shorter than the standard C-C bond length.

MM2 Constants

The MM2 Constants table (MM2 Constants.xml) contains parameters which Chem3D uses to compute the MM2 force field.

Cubic and Quartic Stretch Constants

Integrating the Hooke's Law equation provides the Hooke's Law potential function which describes the potential energy of the ball and spring model. The shape of this potential function is the classical potential well.

$$-\frac{dV}{dx} = F = -dx$$

The Hooke's Law potential function is quadratic, thus the potential well created is symmetrical. The real shape of the potential well is asymmetric and is defined by a complicated function called the Morse Function, but the Hooke's Law potential function works well for most molecules.

$$V(x) = \oint_0^x dV = k\oint_0^x x\,dx = \frac{1}{2}kx^2$$

Certain molecules contain long bonds which are not described well by Hooke's Law. For this reason the MM2 force field contains a cubic stretch term. The cubic stretch term allows for an asymmetric shape of the potential well, thereby allowing these long bonds to be handled. However, the cubic stretch term is not sufficient to handle abnormally long bonds. Thus the MM2 force field contains a quartic stretch term to correct for problems caused by these abnormally long bonds.

Type 2 (-CHR-) Bending Force Parameters for C-C-C Angles

-CHR- Bending K for 1-1-1 angles -CHR- Bending K for 1-1-1 angles in 4-membered rings -CHR- Bending K for 22-22-22 angles in 3-membered rings

These constants are distinct from the force constants specified in the Angle Bending table. The bending force constant (K) for the 1-1-1 angle (1 is the atom type number for the C Alkane atom type) listed in the MM2 Angle Bending parameters table is for an alkane carbon with two non-hydrogen groups attached. Angle bending parameters for carbons with one or two attached hydrogens differ from those for carbons with no attached hydrogens. Because carbons with one or two attached hydrogens frequently occur, separate force constants are used for these bond angles.

The -CHR- Bending K for 1-1-1 angles allows more accurate force constants to be specified for the Type 1 (-CH2-) and Type 2 (-CHR-) interactions. In addition, the -CHR- Bending K for 1-1-1 angles in

4-membered rings and the -CHR- Bending K for 22-22-22 angles (22 is the atom type number for the C Cyclopropane atom type) in 3-membered rings differ from the aforementioned -CHR- Bending K for 1-1-1 angles and thus require separate constants to be accurately specified.

Stretch-Bend Parameters

X-B,C,N,O-Y Stretch-Bend interaction force constant X-B,C,N,O-H Stretch-Bend interaction force constant X-Al,S-Y Stretch-Bend force constant X-Al,S-H Stretch-Bend force constant X-Si,P-Y Stretch-Bend force constant X-Si,P-H Stretch-Bend force constant X-Ga,Ge,As,Se-Y Stretch-Bend force constant

The stretch-bend parameters are force constants for the stretch-bend interaction terms in the prior list of elements. X and Y represent any non-hydrogen atom.

When an angle is compressed, the MM2 force field uses the stretch-bend force constants to lengthen the bonds from the central atom in the angle to the other two atoms in the angle.

For example, the normal C-C-C bond angle in cyclobutane is 88.0°, as compared to a C-C-C bond angle of 110.8° in cyclohexane. The stretch-bend force constants are used to lengthen the C-C bonds in cyclobutane to 1.550Å, from a C-C bond length of 1.536Å in cyclohexane.

Sextic Bending Constant

Sextic bending constant ($*10_{**}8$)

Chem3D uses the sextic bending constant to increase the energy of angles with large deformations from their ideal value.

Dielectric Constants

Dielectric constant for charges Dielectric constant for dipoles

The dielectric constants perform as inverse proportionality constants in the electrostatic energy terms. The constants for the charge and dipole terms are supplied separately so that either can be partially or completely suppressed.

The charge-dipole interaction uses the geometric mean of the charge and dipole dielectric constants.

For example, when you increase the Dielectric constant for dipoles, a decrease in the Dipole/Dipole energy occurs. This has the effect of reducing the contribution of dipole-dipole interactions to the total steric energy of a molecule.

Electrostatic and van der Waals Cutoff Parameters

Cutoff distance for charge/charge interactions Cutoff distance for charge/dipole interactions Cutoff distance for dipole/dipole interactions Cutoff distance for van der Waals interactions

These parameters define the minimum distance at which the fifth-order polynomial switching function is used for the computation of the listed interactions.

MM2 Atom Types

The MM2 Atom Types table (MM2 Atom Types.xml) contains the van der Waals parameters used to compute the force field for each atom in your model.

Each MM2 Atom Type record contains eight fields: Atom type number, R*, Eps, Reduct, Atomic Weight, Lone Pairs, Quality, and Reference.

Atom type number

The Atom Type number field is the atom type to which the rest of the MM2 Atom Type Parameter record applies. The records in the MM2 Atom Type table window are sorted in ascending order of Atom Type Atom type number.

R*

The R* field is the van der Waals radius of the particular atom. The larger the van der Waals radius of an atom is, the larger that atom.

NOTE: *Chem3D uses the van der Waals radius, R*, in the MM2 Atom Types table for computation. It is not the same as the van der Waals radius in the Atom Types table, which is used for displaying the model.*

Eps

The Eps or Epsilon field is a constant which is proportional to the depth of the potential well. As the value of epsilon increases, the depth of the potential well increases, as does the strength of the repulsive and attractive interactions between this atom and other atoms.

NOTE: *For specific VDW interactions, the R^* and Eps values from the VDW Interactions table are used instead of values in the MM2 Atom Types table. See "VDW Interactions" later in the chapter for more information.*

Reduct

Reduct, the fourth field, is a constant used to orient the center of the electron cloud on a hydrogen atom toward the nucleus of the carbon atom to which it is bonded by approximately 10% of the distance between the two atoms.

Any atom in a van der Waals potential function must possess a spherical electron cloud centered about its nucleus. For most larger atoms this is a reasonable assumption, but for smaller atoms such as hydrogen it is not a good assumption. Molecular mechanics calculations based on spherical electron clouds centered about hydrogen nuclei do not give accurate results.

However, it is a reasonable compromise to assume that the electron cloud about hydrogen is still spherical, but that it is no longer centered on the hydrogen nucleus. The Reduct constant is multiplied by the normal bond length to give a new bond length which represents the center of the repositioned electron cloud.

The value of the Reduct field for all non-hydrogen atoms is zero.

Atomic Weight

The fifth field, Atomic Weight, is the atomic weight of atoms represented by this atom type number.

NOTE: *The atomic weight is for the isotopically pure element, i.e. the atomic weight for atom type number 1 is 12.000, the atomic weight of ^{12}C.*

Lone Pairs

The Lone Pairs field contains the number of lone pairs around a particular atom type. Notice that an amine nitrogen, atom type number 8, has one lone pair and an ether oxygen, atom type number 6, has two lone pairs. Lone pairs are treated explicitly for atoms such as these, which have distinctly non-spherical electron distributions. For atom types such as O Carbonyl, which have more nearly spherical electron distributions, no explicit lone pairs are necessary.

NOTE: *Lone pairs are added automatically to atoms which require them at the beginning of an MM2 computation.*

Torsional Parameters

The Torsional Parameters table (Torsional Parameters.xml) contains parameters used to compute the portions of the MM2 force field for the torsional angles in your model. The 4-

Membered Ring Torsional Parameters (4-membered Ring Torsionals.xml) contains torsional parameters for atoms in 4-membered rings.

Each of the records in the Torsional Parameters table and the 4-Membered Ring Torsional Parameters table consists of six fields: Dihedral Type, V1, V2, V3, Quality, and Reference.

Dihedral Type

The Dihedral Type field contains the atom type numbers of the four atom types which describe the dihedral angle.

For example, angle type 1-2-2-1 is a dihedral angle formed by an alkane carbon bonded to an alkene carbon which is first bonded to a second alkene carbon which is bonded to another alkane carbon. In other words, angle type 1-2-2-1 is the dihedral angle between the two methyl groups of 2-butene.

The two alkene carbons are the central atoms of the dihedral angle.

V1

The V1, or 360° Periodicity Torsional constant, field contains the first of three principal torsional constants used to compute the total torsional energy in a molecule. V1 derives its name from the fact that a torsional constant of 360° periodicity can have only one torsional energy minimum and one torsional energy maximum within a 360° period. The period starts at -180° and ends at 180°.

A positive value of V1 means that a maximum occurs at 0° and a minimum occurs at ±180° in a 360° period. A negative value of V1 means that a minimum occurs at 0° and a maximum occurs at ±180° in a 360° period. The significance of V1 is explained in the example following the V2 discussion.

V2

The V2, or 180° Periodicity Torsional constant, field contains the second of three principal torsional constants used to compute the total torsional energy in a molecule. V2 derives its name from the fact that a torsional constant of 180° periodicity can have only two torsional energy minima and two torsional energy maxima within a 360° period.

A positive value of V2 indicates there are minima at 0° and +180°, and there are maxima at -90° and +90° in a 360° period. A negative value of V2 causes the position of the maxima and minima to be switched, as in the case of V1 above. The significance of V2 is explained in the following example.

A good example of the significance of the V1 and V2 torsional constants exists in the 1-2-2-1 torsional parameter of 2-butene. The values of V1 and V2 in the Torsional Parameters table are -0.100 and 10.000 respectively.

Because a positive value of V2 indicates that there are minima at 0° and +180°, these minima signify cis-2-butene and trans-2-butene respectively. Notice that V2 for torsional parameters involving torsions about carbon-carbon double bonds all have values ranging from approximately V2=8.000 to V2=16.250. In addition, V2 torsional parameters involving torsions about carbon-carbon single bonds all have values ranging from approximately V2=-2.000 to V2=0.950.

The values of V2 for torsions about carbon-carbon double bonds are higher than those values for torsions about carbon-carbon single bonds. A consequence of this difference in V2 values is that the energy barrier for rotations about double bonds is much higher than the barrier for rotations about single bonds.

The V1 torsional constant creates a torsional energy difference between the conformations represented by the two torsional energy minima of the V2 constant. As discussed previously, a negative value of V1 means that a torsional energy minimum occurs at 0° and a torsional energy maximum occurs at 180°. The value of V1=-0.100 means that cis-2-butene is a torsional energy minimum that is 0.100 kcal/mole lower in energy than the torsional energy maximum represented by trans-2-butene.

The counterintuitive fact that the V1 field is negative can be understood by remembering that only the total energy can be compared to experimental results. In fact, the total energy of trans-2-butene is computed to be 1.423 kcal/mole lower than the total energy of cis-2-butene. This corresponds closely with experimental results. The negative V1 term has been introduced to compensate for an overestimation of the energy difference based solely on van der Waals repulsion between the methyl groups and hydrogens on opposite ends of the double bond. This example illustrates an important lesson:

There is not necessarily any correspondence between the value of a particular parameter used in MM2 calculations and value of a particular physical property of a molecule.

V3

The V3, or 120° Periodicity Torsional constant, field contains the third of three principal torsional constants used to compute the total torsional energy in a molecule. V3 derives its name from the fact that a torsional constant of 120° periodicity can have three torsional energy minima and three torsional energy maxima within a 360° period. A positive value of V3 indicates there are minima at -60°, +60° and +180° and there are maxima at -120°, 0°, and +120° in a 360° period. A negative value of V3 causes the position of the maxima and minima to be reversed, as in the case of V1 and V2 above. The significance of V3 is explained in the following example.

The 1-1-1-1 torsional parameter of n-butane is an example of the V3 torsional constant. The values of V1, V2 and V3 in the Torsional Parameters table are 0.200, 0.270 and 0.093 respectively. Because a positive value of V3 indicates that there are minima at -60°, +60° and +180° and there are maxima at -120°, 0°, and +120°, the minima at ±60° signify the two conformations of n-butane in which the methyl groups are gauche to one another. The +180° minimum represents the conformation in which the methyl groups are anti to one another. The maximum at 0° represents the conformation in which the methyl groups are eclipsed. The maxima at ±120° conform n-butane in which a methyl group and a hydrogen are eclipsed.

The V1 and V2 torsional constants in this example affect the torsional energy in a similar way to the V1 torsional constant for torsions about a carbon-carbon double bond (see previous example).

NOTE: *The results of MM2 calculations on hydrocarbons do not correspond well with the experimental data on hydrocarbons when only the V3 torsional constant is used (when V1 and V2 are set to zero). However, including small values for the V1 and V2 torsional constants in the MM2 calculations for hydrocarbons dramatically improve the correspondence of the MM2 results with experimental results. This use of V1 and V2 provides little correspondence to any particular physical property of hydrocarbons.*

Record Order

When sorted by Dihedral Angle, the order of the records in the Torsional Parameters table and the 4-Membered Ring Torsional Parameters table is as follows:

1. Records are sorted by the second atom type number in the Dihedral Type field. For example, the record for dihedral type 1-1-1-1 is listed before the record for dihedral type 1-2-1-1.
2. For records where the second atom type number is the same, the records are sorted by the third atom type number in the Dihedral Type field. For example, the record for dihedral type 1-1-1-1 is listed before the record for dihedral type 1-1-2-1.
3. For multiple records where the second and third atom type numbers are the same, the records are sorted by the first atom type number in the Dihedral Type field. For example, the record for dihedral type 5-1-3-1 is listed before the record for dihedral type 6-1-3-1.
4. For multiple records where the first, second and third atom type numbers are the same, the records are sorted by the fourth atom type number in the Dihedral Type field. For example, the record for dihedral type 5-1-3-1 is listed before the record for dihedral type 5-1-3-2.

Out-of-Plane Bending

The Out-of-Plane Bending table (Out-of-Plane Bending Parameters.xml) contains parameters which are used to ensure that atoms with trigonal planar geometry remain planar in MM2 calculations.

There are four fields in records in the Out-of-Plane Bending Parameters table: Bond Type, Force Constant, Quality and Reference.

Bond Type

The first field is the Bond Type which is described by the atom type numbers of the two bonded atoms.

For example, Bond Type 2-3 is a bond between an alkene carbon and a carbonyl carbon.

Force Constant

The Force Constant field, or the out-of-plane bending constant, field contains a measure of the amount of energy required to cause a trigonal planar atom to bend out-of-plane, i.e., to become non-planar. The larger the value of Force Constant for a particular atom, the more difficult it is to coerce that atom to be non-planar.

Record Order

When sorted by Bond Type, the order of the records in the Out-of-Plane Bending Parameters table is as follows:

1. Records are sorted by the first atom type number in the Bond Type field. For example, the record for bond type 2-1 is before the record for bond type 3-1.
2. For records where the first atom type number is the same, the records are sorted by the second atom type number in the Bond Type field. For example, the record for bond type 2-1 is before the record for bond type 2-2.

NOTE: *Out-of-plane bending parameters are not symmetrical. For example, the force constant for a 2-3 bond refers to the plane about the type 2 atom. The force constant for a 3-2 bond refers to the plane about the type 3 atom.*

VDW Interactions

The parameters contained in the VDW parameters table (VDW Interaction.xml) are used to adjust specific VDW interactions in a molecule, such as hydrogen bonding, to provide better correspondence with experimental data in calculating the MM2 force field.

For example, consider the VDW interaction between an Alkane carbon (Atom Type 1) and a hydrogen (Atom Type 5). Normally, the VDW energy is based on the sum of the VDW radii for these atoms, found for each atom in the Atom Types table (1.900Å for Atom type number 1 + 1.400Å for Atom type number 2 = 3.400Å). However, better correspondence between the computed VDW energy and experimental data is found by substituting this sum with the value found in the VDW Interactions table for this specific atom type pair (Atom Types 1-5 = 3.340Å).

Similarly, an Eps parameter is substituted for the geometric mean of the Eps parameters for a pair of atoms if their atom types appear in the VDW Interactions table.

Record Order

When sorted by Atom Type, the order of the records in VDW Interactions table window is as follows:

Records are sorted by the first atom type number in the Atom Type field. For example, the record for Atom Type 1-36 is before the record for atom type 2-21.

For records where the first atom type number is the same, the records are sorted by the second atom type number in the Atom Type field. For example, the record for atom type 2-21 is before the record for atom type 2-23.

Appendix I: MM2

Overview

This appendix contains miscellaneous information about the MM2 parameters and force field.

MM2 Parameters

The original MM2 parameters include the elements commonly used in organic compounds: carbon, hydrogen, nitrogen, oxygen, sulfur and halogens. The atom type numbers for these atom types range from 1 to 50.

The MM2 parameters were derived from three sources:

1. Most of the parameters were provided by Dr. N. L. Allinger.
2. Several additional parameters were provided by Dr. Jay Ponder, author of the TINKER program.
3. Some commonly used parameters that were not provided by Dr. Allinger or Dr. Ponder are provided by CambridgeSoft Corporation. However, most of these parameters are estimates which are extrapolated from other parameters.

The best source of information on the MM2 parameter set is *Molecular Mechanics*, Burkert, Ulrich and Allinger, Norman L., ACS Monograph 177, American Chemical Society, Washington, DC, 1982.

A method for developing reasonable guesses for parameters for non-MM2 atom types can be found in "Development of an Internal Searching Algorithm for Parameterization of the MM2/MM3 Force Fields", Journal of Computational Chemistry, Vol 12, No. 7, 844-849 (1991).

Other Parameters

The rest of the parameters consist of atom types and elements in the periodic table which were not included in the original MM2 force field, such as metals. The rectification type of all the non-MM2 atom types in the Chem3D Parameter tables is Hydrogen (H). The atom type numbers for these atom types range from 111 to 851. The atom type number for each of the non-MM2 atom types in the MM2 Atom Type Parameters table is based on the atomic number of the element and the number of ligands in the geometry for that atom type. To determine an atom type number, the atomic number is multiplied by ten, and the number of ligands is added.

For example, Co Octahedral has an atomic number of 27 and six ligands. Therefore the atom type number is 276.

In a case where different atom types of the same element have the same number of ligands (Iridium Tetrahedral, Atom Type # 774 and Iridium Square Planar, Atom Type # 779), the number nine is used for the second geometry.

Viewing Parameters

To view the parameters used by Chem3D to perform MM2 computations:

- From the View menu, point to Parameter Tables, and choose a table.

  The table you chose opens in a window.

Editing Parameters

You can edit the parameters that come with Chem3D. Parameters that you add or change can be guesses or approximations that you make, or values obtained from current literature.

In addition, there are several adjustable parameters available in the MM2 Constants table. For information on parameters and MM2 constants, see "The Force-Field" on page 136.

NOTE: *Before performing any editing we strongly recommend that you create back-up copies of all the parameter files located in the C3DTable directory.*

To add a new parameter to the Torsional parameters table:

1. From the View menu, point to Parameter Tables and choose Torsional Parameters.

   The Torsional Parameters table opens in a window.
2. Enter the appropriate data in each field of the parameter table. Be sure that the name for the parameter is not duplicated elsewhere in the table.
3. Close and Save the table.

The MM2 Force Field in Chem3D

Chem3D includes a new implementation of Norman L. Allinger's MM2 force field based in large measure on work done by Jay W. Ponder of Washington University. This appendix does not attempt to completely describe the MM2 force field, but discusses the way in which the MM2 force field is implemented and used in Chem3D and the differences between this implementation, Allinger's MM2 program (QCPE 395), and Ponder's TINKER system (M.J. Dudek and J.W. Ponder, *J. Comput. Chem.*, **16**, 791-816 (1995)).

For a review of MM2 and applications of molecular mechanics methods in general, see *Molecular Mechanics*, by U. Burkert and N. L. Allinger, ACS, Washington, D.C., USA, 1982. *Computational Chemistry*, by T. Clark, Wiley, N.Y., USA, 1985, also contains an excellent description of molecular mechanics.

For a description of the TINKER system and the detailed rationale for Ponder's additions to the MM2 force field, visit the TINKER home page at http://dasher.wustl.edu/tinker.

For a description and review of molecular dynamics, see *Dynamics of Proteins and Nucleic Acids*, J. Andrew McCammon and Stephen Harvey, Cambridge University Press, Cambridge, UK, 1987. Despite its focus on biopolymers, this book contains a cogent description of molecular dynamics and related methods, as well as information applicable to other molecules.

Chem3D Changes to Allinger's Force Field

The Chem3D implementation of the Allinger Force Field differs in these areas:

1. A charge-dipole interaction term
2. A quartic stretching term
3. Cutoffs for electrostatic and van der Waals terms with a fifth-order polynomial switching function
4. Automatic pi system calculation when necessary

Charge-Dipole Interaction Term

Allinger's potential function includes one of two possible electrostatic terms: one based on bond dipoles, or one based on partial atomic charges. The addition of a charge-dipole interaction term allows for a combined approach, where partial charges are represented as bond dipoles, and charged groups, such as ammonium or phosphate, are treated as point charges.

Quartic Stretching Term

With the addition of a quartic bond stretching term, troublesome negative bond stretching energies which appear when long bonds are treated by Allinger's force field are eliminated.

The quartic bond stretching term is required primarily for molecular dynamics; it has little or no effect on low energy conformations.

To precisely reproduce energies obtained with Allinger's force field:

- Set the quartic stretching constant in the MM2 Constants table window to zero.

  The quartic term is eliminated.

Electrostatic and van der Waals Cutoff Terms

The cutoffs for electrostatic and van der Waals terms greatly improve the computation speed for large molecules by eliminating long range interactions from the computation.

To precisely reproduce energies obtained with Allinger's force field:

- Set the cutoff distances to large values (greater than the diameter of the model).

  Every interaction is then computed.

The cutoff is implemented gradually, beginning at 50% of the specified cutoff distance for charge and charge-dipole interactions, 75% for dipole-dipole interactions, and 90% for van der Waals interactions. Chem3D uses a fifth-order polynomial switching function so that the resulting force field is second-order continuous.

Because the charge-charge interaction energy between two point charges separated by a distance r is proportional to 1/r, the charge-charge cutoff must be rather large, typically 30 or 40Å. The charge-dipole, dipole-dipole, and van der Waals energies, which fall off as $1/r^2$, $1/r^3$, and $1/r^6$, respectively, can be cut off at much shorter distances, for example, 25Å, 18Å, and 10Å, respectively. Fortunately, since the van der Waals interactions are by far the most numerous, this cutoff speeds the computation significantly, even for relatively small molecules.

Pi Orbital SCF Computation

Chem3D determines whether the model contains any pi systems, and performs a Pariser-Parr-Pople pi orbital SCF computation for each system. A pi system is defined as a sequence of three or more atoms of types which appear in the Pi Atoms table window (PIATOMS.xml).

The method used is that of D.H. Lo and M.A. Whitehead, *Can. J. Chem.*, 46, 2027 (1968), with heterocycle parameters according to G.D. Zeiss and M.A. Whitehead, *J. Chem. Soc. (A)*, 1727 (1971). The SCF computation yields bond orders which are used to scale the bond stretching force constants, standard bond lengths, and twofold torsional barriers.

A step-wise overview of the process used to do pi system calculations is as follows:

5. A matrix called the Fock matrix is initialized to represent the favorability of sharing electrons between pairs of atoms in a pi system.

6. The pi molecular orbitals are computed from the Fock matrix.
7. The pi molecular orbitals are used to compute a new Fock matrix, then this new Fock matrix is used to compute better pi molecular orbitals.
8. step 6 and Step 7 are repeated until the computation of Fock matrix and the pi molecular orbitals converge. This method is called the self-consistent field technique or a pi-SCF calculation.
9. A pi bond order is computed from the pi molecular orbitals.
10. The pi bond order is used to modify the bond length (BL_{res}) and force constant (KS_{res}) for each sigma bond in the pi system.
11. The values of KS_{res} and BL_{res} are used in the molecular mechanics portion of the MM2 computation to further refine the molecule.

To examine the computed bond orders after an MM2 computation:

1. In the Pop-up Information control panel, select Bond Order.
2. Position the pointer over a bond.

The information box contains the newly computed bond orders for any bonds that are in a pi system.

Appendix J: MOPAC

Overview

The appendix contains miscellaneous information about MOPAC.

You can find additional information about MOPAC by visiting the MOPAC home page at:

http://www.cachesoftware.com/mopac/index.shtml

MOPAC Background

MOPAC was created by Dr. James Stewart at the University of Texas in the 1980s. It implements semi-empirical methodologies for analyzing molecular models. (MOPAC stands for Molecular Orbital PACkage.) Due to its complexity and command line user interface, its use was limited until the mid 1990s.

Since version 3.5 (1996), Chem3D has provided an easy-to-use GUI interface for MOPAC that makes it accessible to the novice molecular modeller, as well as providing greater usability for the veteran modeller. We are currently supporting MOPAC 2000.

MOPAC 2000 is copyrighted by Fujitsu, Ltd.CS MOPAC is the licensed version that runs under Chem3D.

Potential Functions Parameters

MOPAC provides five potential energy functions: MINDO/3, MNDO, PM3, AM1, and MNDO-d. All are SCF (Self Consistent Field) methods. Each function represents an approximation in the mathematics for solving the Electronic Schrödinger equation for a molecule.

Historically, these approximations were made to allow *ab initio* calculations to be within the reach of available computer technology. Currently, *ab initio* methods for small molecules are within the reach of desktop computers. Larger molecules, however, are still more efficiently modeled on the desktop using semi-empirical or molecular mechanics methodologies.

To understand the place that the potential energy functions in MOPAC take in the semi-empirical arena, here is a brief chronology of the approximations that comprise the semi-empirical methods. The first approximation was termed CNDO for Complete Neglect of Differential Overlap. The next approximation was termed INDO for Intermediate Neglect of Differential Overlap, Next followed MINDO/3, which stands for "Modified Intermediate Neglect of Differential Overlap". Next was MNDO, which is short for "Modified Neglect of Differential Overlap" which corrected MINDO/3 for various organic molecules made up from elements in rows 1 and 2 of the periodic table. AM1 improved upon MNDO markedly. Finally the most recent, PM3 is a reparameterization of AM1. The approximations in PM3 are the same as AM1.

This sequence of potential energy functions represents a series of improvements to support the initial assumption that complete neglect of diatomic orbitals would yield useful data when molecules proved too resource intensive for *ab initio* methods.

Adding Parameters to MOPAC

Parameters are in constant development for use with PM3 and AM1 potential functions. If you find that the standard set of parameters that comes with CS MOPAC does not cover an element that you need, for example Cu, you can search the literature for the necessary parameter and add it at run time when performing a MOPAC job. This flexibility greatly enhances the usefulness of MOPAC.

You can add parameters at run time using the keyword EXTERNAL=name, where name is the name of the file (and its full path) containing the additional parameters.

A description of the required format for this file can be found in Figure 3.4, page 43 of the MOPAC 2000 V.1.3 manual included on the CD-ROM.

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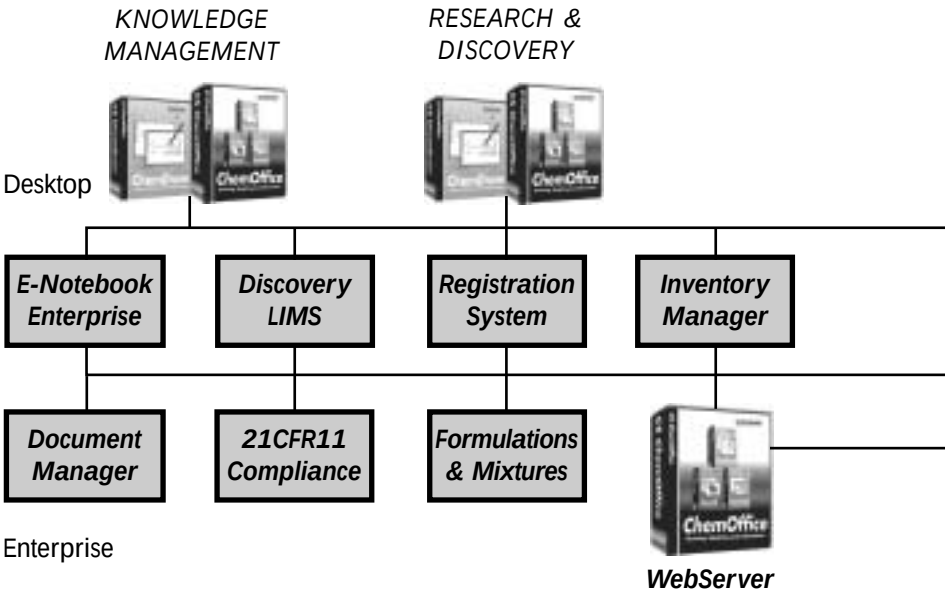


DESKTOP SOFTWARE

ChemOffice
E-Notebook
ChemDraw
Chem3D
ChemFinder
ChemInfo

Success begins at the desktop, where scientists use *ChemDraw* and *ChemOffice* to pursue their ideas and communicate with colleagues using the natural language of chemical structures, models, and information. In the lab, scientists capture their results by organizing chemical information, documents, and data with *E-Notebook*. *Chem3D* modeling and *ChemFinder* information retrieval integrate smoothly with *ChemOffice* and Microsoft Office to speed day-to-day research tasks.

ENTERPRISE SOLUTIONS

ChemOffice WebServer
Oracle Cartridge

Just as *ChemOffice* supports the daily work of the individual scientist, enterprise solutions and databases, built on *ChemOffice WebServer,* and *Oracle Cartridge* help organizations collaborate and share information.

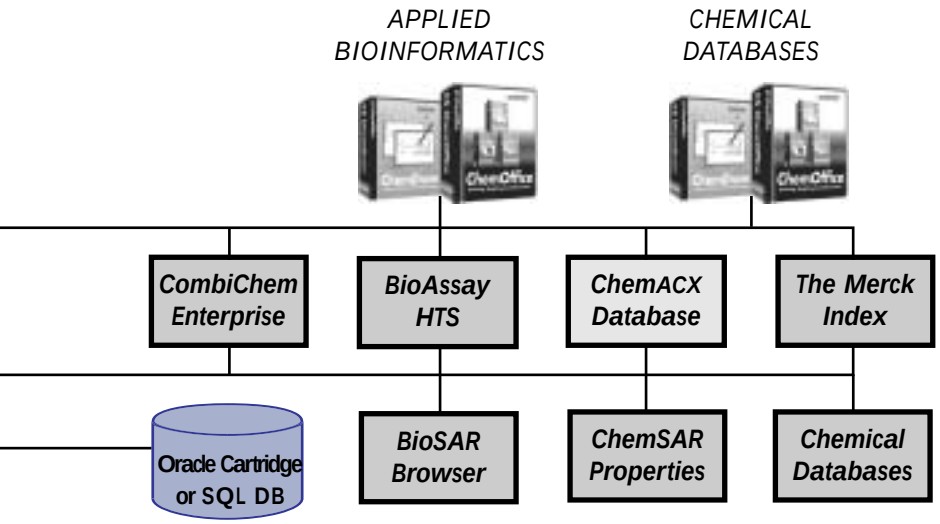
KNOWLEDGE MANAGEMENT

E-Notebook Enterprise
Document Manager
Discovery LIMS
21CFR11 Compliance

Research organizations thrive when information is easily captured, well organized, and available to others who need it. *E-Notebook Enterprise* streamlines daily record keeping with rigorous security and efficient archiving, and facilitates searches by text and structure. *Document Manager* organizes procedures and reports for archiving and chemically-intelligent data mining. *Discovery LIMS* tracks laboratory requests, and *21CFR11 Compliance* implements an organization's regulatory compliance processes.

SOLUTIONS

Enterprise Solutions



RESEARCH & DISCOVERY

Registration System
Formulations & Mixtures
Inventory Manager
CombiChem Enterprise

Managing the huge data streams of new lab technology is a key challenge. *Registration System* organizes information about new compounds according to an organization's business rules, while *Inventory Manager* works with *Registration System* and chemical databases for complete management of chemical inventories. *CombiChem Enterprise* and *Formulations & Mixtures* are also important parts of research data management.

APPLIED BIOINFORMATICS

BioAssay HTS
BioSAR Browser

Finding structural determinants of biological activity requires processing masses of biological assay data. Scientists use *BioAssay HTS* and *BioSAR Browser* to set up biological models and visualize information, to generate spreadsheets correlating structure and activity, and to search by structure.

CHEMICAL DATABASES

ChemACX Database
ChemSAR Properties
The Merck Index
Chemical Databases

Good research depends on reference information, starting with the structure-searchable *ChemACX Database* of commercially available chemicals. *The Merck Index* 13th Edition and other databases provide necessary background about chemicals, their properties, and reactions.

CONSULTING & SERVICES

Consulting Development
Support & Training

CambridgeSoft's scientific staff has the industry experience, and chemical and biological knowledge to maximize the effectiveness of your information systems.

CS ChemOffice

	Software Suites	ChemOffice Ultra	ChemOffice Pro	ChemDraw Ultra	ChemDraw Pro	ChemDraw Std	Chem3D Ultra	E-Notebook Ultra
	Includes							
Software	*ChemDraw Ultra	Win/Mac	■	■	■				
	*ChemDraw Pro	Win/Mac				■			
	*ChemDraw Std	Win/Mac					■	■	■
	*ChemDraw Plugin Pro	Win/Mac	■	■	■	■			
	*Chem3D Ultra	Win	■					■	
	*Chem3D Pro	Win		■					
	Chem3D Std	Win			■				■
	*Chem3D Plugin Pro	Win	■	■	■			■	
	*E-Notebook Ultra	Win	■						■
	ChemFinder Pro	Win	■	■					■
	ChemFinder Std	Win			■			■	
Applications & Features	ChemDraw/Spotfire	Win	■						
	*BioAssay Pro	Win	■						
	Purchase/Excel	Win	■						
	CombiChem/Excel	Win	■	■	■				■
	ChemFinder/Office	Win	■	■	■				■
	ChemDraw/Excel	Win	■	■	■				■
	Name=Struct	Win/Mac	■	■	■				
	Struct=Name	Win/Mac	■	■	■				
	ChemNMR	Win/Mac	■	■	■				
	CLogP/ChemDraw	Win/Mac	■	■	■				
	BioArt	Win/Mac	■	■	■				
	Structure Clean Up	Win/Mac	■	■	■	■			
	Polymer Draw	Win/Mac	■	■	■	■			
	LabArt	Win/Mac	■	■	■	■	■	■	■
	ChemSAR/Excel	Win	■	■				■	
	3D Query	Win	■	■					
	MOPAC/Chem3D	Win	■					■	
	GAMESS Client	Win	■					■	
	Gaussian Client	Win	■					■	
	Tinker/Chem3D	Win	■					■	
	*CAMEO/ChemDraw	Win							
Databases	*The Merck Index	Win	■						
	*ChemACX Ultra	Win	■						
	ChemSCX	Win	■						
	ChemMSDX	Win	■						
	*ChemINDEX Ultra	Win	■	■					■
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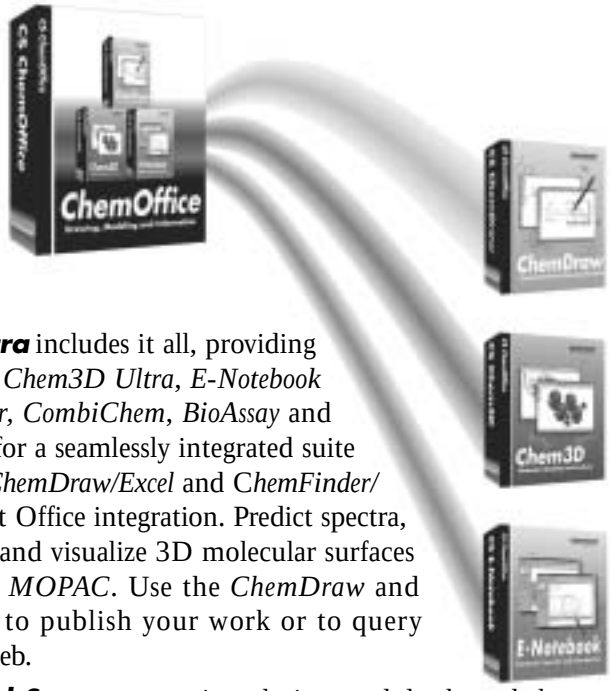
*Available Separately

Desktop to Enterprise Solutions



ChemOffice Ultra includes it all, providing *ChemDraw Ultra, Chem3D Ultra, E-Notebook Ultra, ChemFinder, CombiChem, BioAssay* and *The Merck Index*, for a seamlessly integrated suite for chemists.Use *ChemDraw/Excel* and *ChemFinder/Word* for Microsoft Office integration. Predict spectra, use *Name=Struct*, and visualize 3D molecular surfaces and orbitals with *MOPAC*. Use the *ChemDraw* and *Chem3D Plugins* to publish your work or to query databases on the web.

ChemOffice WebServer enterprise solutions and databases help organizations collaborate on shared information with *ChemDraw* web-based interface and *Oracle Cartridge* security.

Knowledge Management with *E-Notebook Enterprise* streamlines daily record-keeping with rigorous security and efficient archiving. *Document Manager* indexes chemical structure content of documents and folders.

Research & Discovery efforts are improved with *Registration System* by organizing new compound information, while *Inventory Manager* works with chemical databases for complete management of chemical inventories.

Applied BioInformatics scientists use *BioAssay HTS* and *BioSAR Browser* to set up biological models and visualize information, to generate spreadsheets correlating structure and activity, and to search by structure.

Chemical Databases include the *ChemACX Database* of commercially available chemicals, *The Merck Index* 13th edition, and other databases.

Consulting & Services includes consulting development, technical support, and education training for pharmaceutical, biotechnology, and chemical customers, including government and education, by CambridgeSoft's experienced staff.

ChemOffice WebServer

Enterprise Solutions & Databases

- *Oracle Cartridge & Database Webserver*

Knowledge Management

- *E-Notebook Enterprise*, *Document Mgr*, *Discovery LIMS & 21CFR11 Compliance*

Research & Discovery

- *Registration System*, *Formulations & Mixtures*, *Inventory Manager & CombiChem Enterprise*

Applied BioInformatics

- *BioAssay HTS & BioSAR Browser*

Chemical Databases

- *The Merck Index*, *ChemACX & ChemSAR Properties*

ChemOffice Ultra

Ultimate Drawing, Modeling & Information

- Adds *The Merck Index, E-Notebook*, *CombiChem*, *MOPAC*, *BioAssay & ChemACX* to *Office Pro*

ChemOffice Pro

Premier Drawing, Modeling & Information

- Includes *ChemDraw Ultra*, *Chem3D Pro*, *ChemSAR/Excel*, *ChemFinder Pro*, *ChemINDEX & ChemRXN* databases

Also Available Separately...

ChemDraw Ultra

Ultimate Drawing, Query & Analysis

- Adds *ChemDraw/Excel, ChemNMR, Name=Struct, AutoNom & ChemFinder / Word* to *ChemDraw Pro*
- *ChemNMR*, Stereochemistry, Polymers & *BioArt*

ChemDraw Pro

Premier Drawing & Database Query

- Define complex database queries
- ISIS/Draw & Base compatible via copy/paste
- *Structure CleanUp* and Chemical Intelligence

Chem3D Ultra

Ultimate Modeling, Visualization & Analysis

- Adds *MOPAC*, *CLogP*, *Tinker, ChemProp*, *ChemSAR & Chem3D Plugin* to *Chem3D Pro*
- Advanced modeling & molecular analysis tool

E-Notebook Ultra

Ultimate Journaling & Information

- *E-Notebook, ChemDraw Std, Chem3D Std, ChemDraw/Excel & CombiChem/Excel*
- Includes *ChemFinder, ChemFinder/Word, ChemINDEX & ChemRXN* databases

Some features are Windows only.
All specifications subject to change without notice.

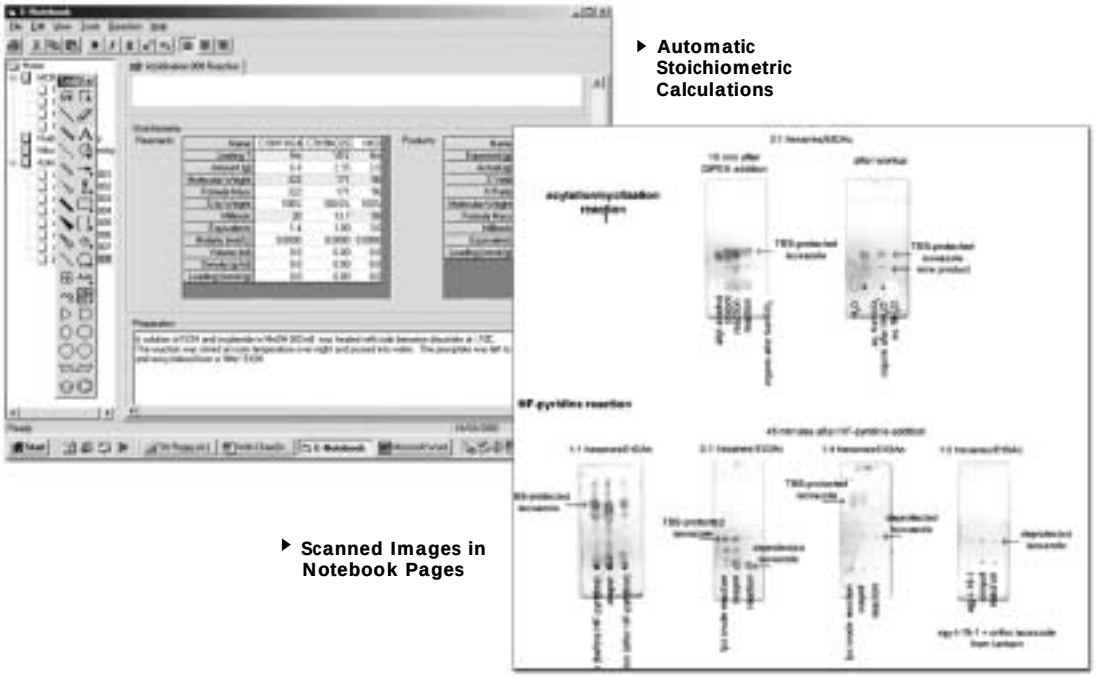
CS E-Notebook

Electronic Journal and Information

E-Notebook Ultra streamlines daily record keeping tasks of research scientists, maintains live chemical structures and data, and saves time documenting work and retrieving chemical information. *E-Notebook* combines all of your notebooks into one and sets up as many project notebooks as you need, organized the way you work. Notebook pages include *ChemDraw* documents, Excel spreadsheets, Word documents and spectral data. *E-Notebook* automatically performs stoichiometry calculations on *ChemDraw* reaction pages. Search by structure, keyword, dates and other types of data. Maintain required hardcopy archives by printing out pages. Information cannot be accidentally modified. Spectral controls from Thermo Galactic are available.

CombiChem/Excel builds combinatorial libraries with embedded *ChemDraw* structures using *ChemDraw/Excel* for Windows. Find reagents with *ChemFinder* and design experiments.

BioAssay Pro, available in *ChemOffice Ultra*, allows for flexible storage and retrieval of biological data. It is designed for complex lead optimization experiments and supports almost any biological model.

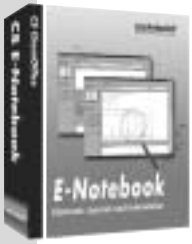


▸ **Automatic Stoichiometric Calculations**

▸ **Scanned Images in Notebook Pages**

E-Notebook Ultra

Ultimate Journaling & Information



- Advanced search and structure query features
- Stores structures and models for easy retrieval
- Stores physical and calculated data
- Search by substructure, including stereochemistry, using *ChemDraw*
- Search and store chemical reaction data
- *CombiChem/Excel* combinatorial libraries
- Integration with *ChemDraw* and *Chem3D*
- Import/export MDL SD & RD files

CombiChem/Excel

Combinatorial Chemistry in Excel

- Generate combinatorial libraries
- Choose starting materials & reaction schemes
- View structures & track plate/well assignments

ChemFinder Pro

Premier Searching & Information

- Advanced search & structure query features
- Stores structures & reactions along with calculated data & associated information
- Search by substructure including stereochemistry using *ChemDraw*
- Integration with *ChemDraw* & *Chem3D*
- Import/export MDL SD & RD files

ChemInfo Std

Reference & Reaction Searching

- *ChemINDEX* for small molecule information
- *ChemRXN* for reaction databases

BioAssay Pro

Biological Assay Structure Activity

- Set up biological models & visualize information
- Search data by structure to isolate key structural determinants of biological activity
- Tabulate & analyze structure-activity relationships with spreadsheet templates
- Available in *ChemOffice Ultra*

SYSTEMS & LANGUAGES

English & Japanese
Windows: 95, 98, Me, NT, 2000, XP
This software is Windows only.
All specifications subject to change without notice.

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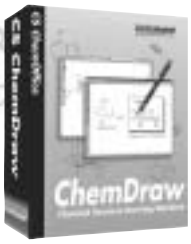
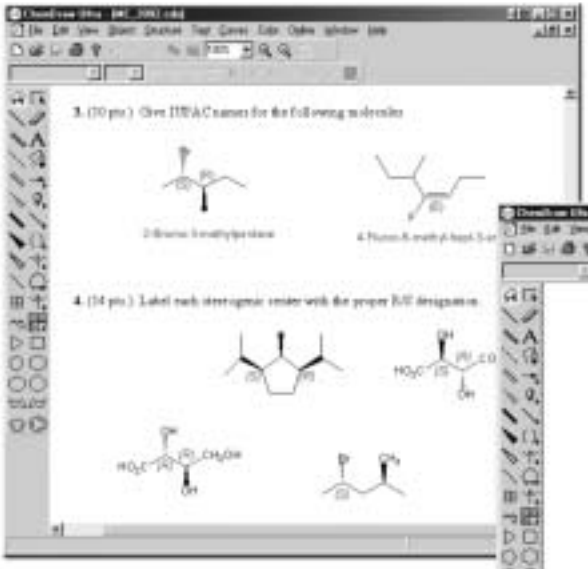
CS ChemDraw

Chemical Structure Drawing Standard

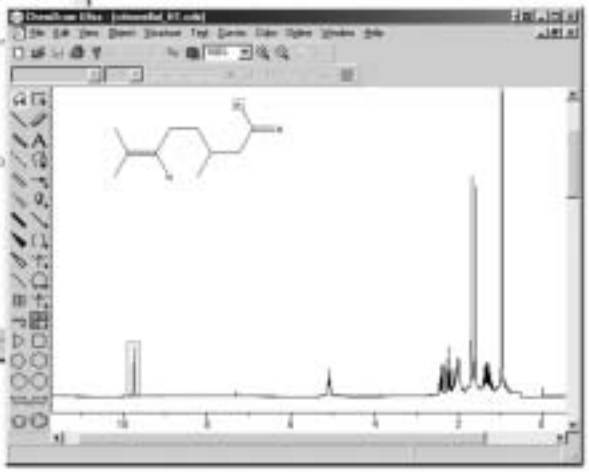


ChemDraw Ultra adds *ChemDraw/Excel*, *ChemNMR*, *Name=Struct*, Beilstein's *AutoNom*, *CLogP* and *ChemFinder/Word* to *ChemDraw Pro*. With rich polymer notation, atom numbering, *BioArt* templates, and modern user interface, *ChemDraw* is more powerful than ever before. Create tables of structures, identify and label stereochemistry, estimate NMR spectra from a *ChemDraw* structure with structure-to-spectrum correlation, obtain structures from chemical names, assign names from structures, and create multi-page documents and posters.

ChemDraw Pro will boost your productivity more than ever. Draw publication-quality structures and reactions. Publish on the web using the *ChemDraw Plugin*. Create precise database queries by specifying atom and bond properties and include stereochemistry. Display spectra, structures, and annotations on the same page. Use the *Online Menu* to query *ChemACX.Com* by structure, identify available vendors, and order online.



▸ **Stereochemistry**



▸ **Structure-to-Spectrum NMR Correlation**

ChemDraw Ultra

Ultimate Drawing, Query & Analysis

- Adds *ChemDraw/Excel, ChemNMR, Name=Struct, AutoNom & ChemFinder/Word* to *ChemDraw Pro*
- *Name=Struct/AutoNom* creates structures from names & vice versa
- *ChemNMR* predicts ^{1}H & ^{13}C NMR line spectra with peak-to-structure correlation
- Polymer notation based on IUPAC standards
- *ChemDraw/Excel* brings chemistry to Excel

ChemDraw Pro

Premier Drawing & Information Query

- Query databases precisely by specifying atom & bond properties, reaction centers, substituent counts, R-groups & substructure
- Read ISIS files with Macintosh/Windows cross-platform compatibility
- *Structure Clean Up* improves poor drawings
- Display spectra from SPC and JCAMP files
- Chemical intelligence includes valence, bonding & atom numbering
- Right-button menus speed access to features

ChemDraw Std

Publication Quality Structure Drawing

- Draw and print structures & reactions in color, and save as PostScript, EPS, GIF, SMILES & more
- Collections of pre-defined structure templates
- Large choice of bonds, arrows, brackets, orbitals, reaction symbols & *LabArt*
- Style templates for most chemical journals
- Compatible with *Chem3D*, *ChemFinder*, *ChemInfo, E-Notebook* & Microsoft Office

ChemDraw Plugin

Advanced WWW Structure Client

- Embed live *ChemDraw* documents in WWW pages
- Works with Netscape & Internet Explorer
- Included with *ChemDraw Ultra & Pro*

SYSTEMS & LANGUAGES

Windows & Macintosh English, Japanese, French, German
Windows: 95, 98, Me, NT, 2000, XP
Macintosh: MacOS 8.6-10.1
Some features are Windows only.
All specifications subject to change without notice.

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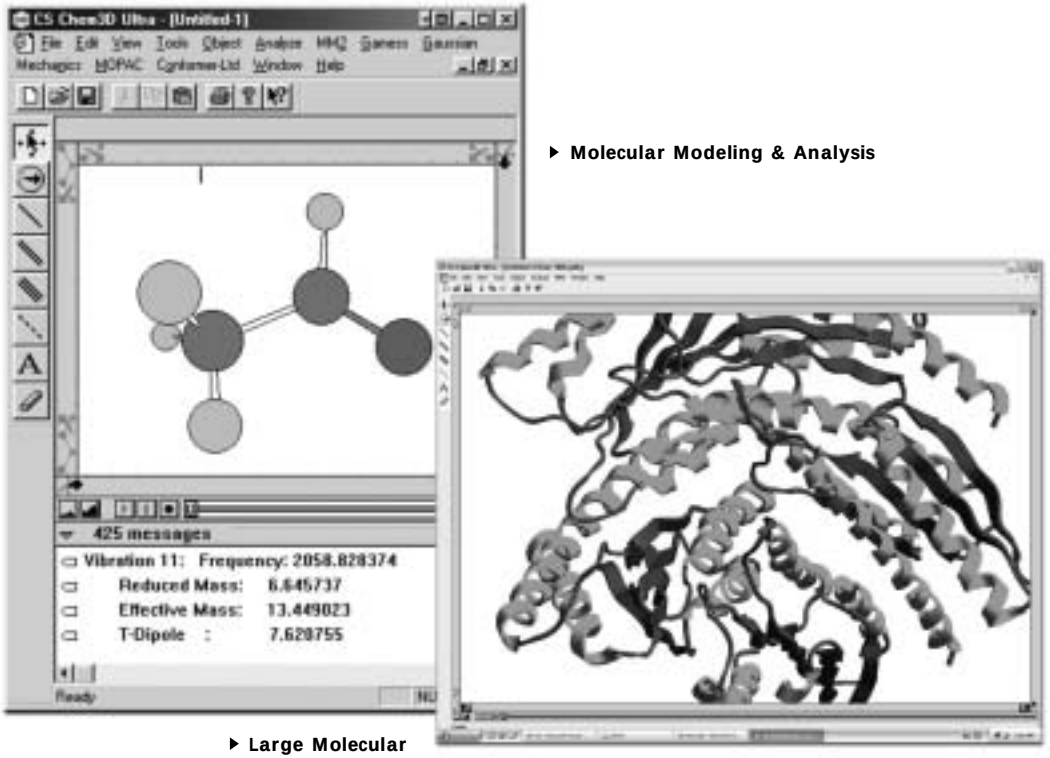
CS Chem3D

Molecular Modeling and Analysis

Chem3D Ultra includes *MOPAC*, *Tinker* and set-up/control interfaces for optional use of GAMESS and Gaussian. Estimate advanced physical properties with *CLogP* and *ChemProp*, and create SAR tables using property servers to generate data for lists of compounds. Use *ChemSAR/Excel* to explore structure activity relationships and use add-on *Conformer* for conformational searching. Publish and view models on the web using the *Chem3D Plugin*.

Chem3D Pro brings workstation quality molecular visualization and display to your desktop. Convert *ChemDraw* and ISIS/Draw sketches into 3D models. View molecular surfaces, orbitals, electrostatic potentials, charge densities and spin densities. Use built-in extended Hückel to compute partial atomic charges. Use MM2 to perform rapid energy minimizations and molecular dynamics simulations. *ChemProp* estimates physical properties such as logP, boiling point, melting point and more. Visualize Connolly surface areas and molecular volumes.



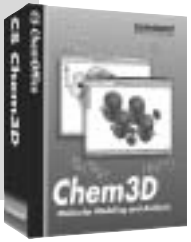
▸ **Molecular Modeling & Analysis**

▸ **Large Molecular Visualization**

Chem3D Ultra

Ultimate Modeling, Visualization & Analysis

- Adds *MOPAC*, *CLogP*, *Tinker, ChemProp*,*ChemSAR & Chem3D Plugin* to *Chem3D Pro*
- Includes GAMESS & Gaussian client interfaces
- *ChemSAR/Excel* builds SAR tables



Chem3D Pro

Premier Modeling, Visualization & Analysis

- Create 3D models from *ChemDraw* or ISIS Draw, accepts output from other modeling packages
- Model types: space filling CPK, ball & stick, stick, ribbons, VDW dot surfaces & wire frame
- Compute & visualize partial charges, 3D surface properties & orbital mapping
- Polypeptide builder with residue recognition
- *ChemProp*—Basic property predictions with Connolly volumes & surface areas
- MM2 minimization & molecular dynamics, extended Hückel MO calculations
- Supports: PDB, MDL Molfile, Beilstein ROSDAL, Tripos SYBYL MOL, EPS, PICT, GIF, 3DMF, TIFF, PNG & more

MOPAC/Chem3D

Advanced Semi-Empirical Computation

- Calculate ΔH_f, solvation energy, dipoles, charges, UHF & RHF spin densities, MEP, charge densities & more
- Optimize transition state geometries
- AM1, PM3, MNDO & MINDO/3 methods

CAMEO/ChemDraw

Synthetic Reaction Prediction

- Expert system predicts and displays products
- *ChemDraw* creates starting materials when you choose reaction conditions; sold separately

Chem3D Plugin

Advanced WWW Model Client

- Works with Microsoft Internet Explorer
- Visualize 3D molecules on *ChemFinder.Com*

SYSTEMS & LANGUAGES

Windows & Macintosh English & Japanese
Windows: 95, 98, Me, NT, 2000, XP
Macintosh: MacOS 8.6-9.2.X
Some features are Windows only.
All specifications subject to change without notice.

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CS ChemFinder

Searching and Information Integration

ChemFinder Pro is a fast, chemically intelligent, relational database search engine for personal, group or enterprise use. Extended integration with Microsoft Excel and Word adds chemical searching and database capability to spreadsheets and documents.

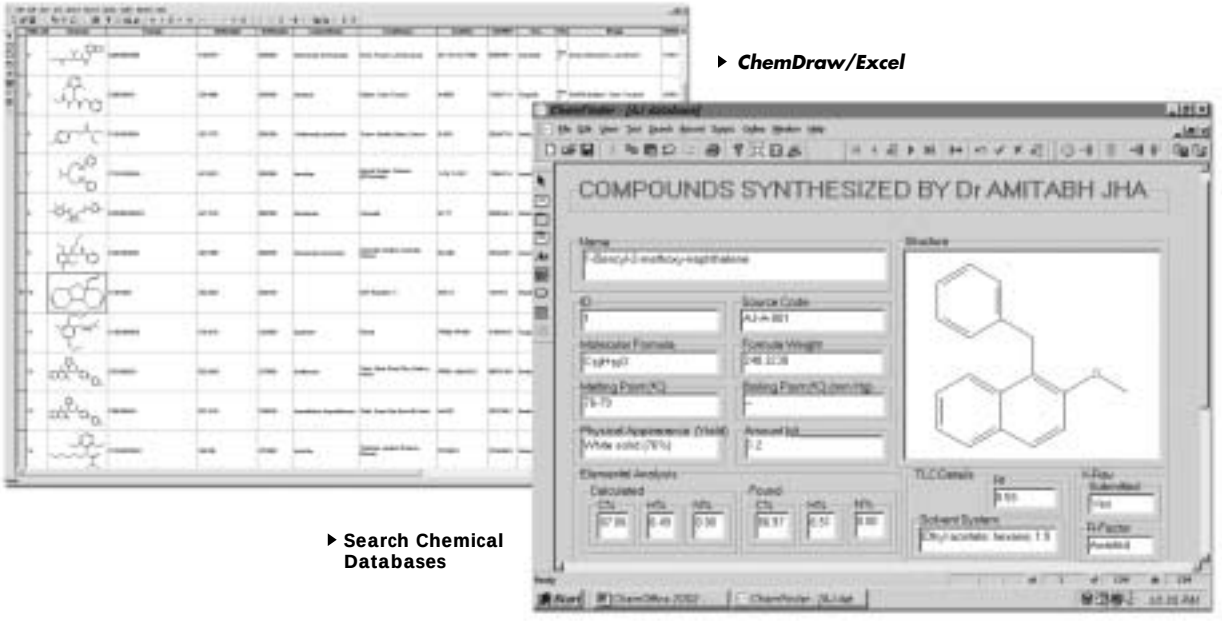
An ever-increasing number of chemical databases are available in *ChemFinder* format. Compatibility with MDL ISIS databases is provided by SDfile and RDfile import/export. *ChemFinder* provides network server workgroup functionality when used with *ChemOffice WebServer.*

ChemFinder/Word is an extension of Microsoft Excel and Word for Windows. Create structure searchable spreadsheets and index documents with embedded *ChemDraw* structures.

ChemDraw/Excel adds chemical intelligence to Microsoft Excel for Windows. Show structures in spreadsheet cells, tabulate chemical calculations and analyze data with Excel functions and graphs.

Purchase/Excel uses *ChemDraw/Excel* to manage reagent lists and track purchasing information.

CombiChem/Excel builds combinatorial libraries with embedded *ChemDraw* structures using *ChemDraw/Excel* for Windows. Find reagents with *ChemFinder* and design experiments.



▸ ***ChemDraw/Excel***

▸ **Search Chemical Databases**

ChemFinder/Word
• Search structures in documents & folders
ChemDraw/Excel
• Add chemical intelligence to spreadsheets
Purchase/Excel
• Organize chemical purchasing information

ChemFinder Pro
Premier Searching & Information
- Advanced search and structure query features
- Stores structures and reactions along with calculated data and associated information
- Search by substructure including stereochemistry using *ChemDraw*
- Import/export MDL SD and RD files
- Integration with *ChemDraw* and *Chem3D*

ChemFinder/Word
Searching Word, Excel & More
- Searches documents for embedded structures
- Indexes structures and source locations
- Searches specified folders and whole hard drives

ChemDraw/Excel
Searching & Calculating in Excel
- Displays *ChemDraw* structures in spreadsheet cells
- Adds chemical calculations to Excel functions
- Useful for graphing and analyzing chemical data

Purchase/Excel
High Throughput Purchasing
- Finds vendor and price information from *ChemACX Database or ChemACX.Com*
- Search for suppliers and purchase online
- Maintains lists of compounds

CombiChem/Excel
Combinatorial Chemistry in Excel
- Generate combinatorial libraries
- Choose starting materials and reaction schemes
- View structures and track plate/well assignments

SYSTEMS & LANGUAGES

English & Japanese
Windows: 95, 98, Me, NT, 2000, XP
This software is Windows only.
All specifications subject to change without notice.

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CS ChemInfo

Reference and Chemical Databases

The Merck Index is an encyclopedia of chemicals, drugs, and biologicals, with over 10,000 monographs covering names, synonyms, physical properties, preparations, patents, literature references, therapeutic uses and more.

ChemACX Pro includes 500,000 chemical products from 300 supplier catalogs, searchable with a single query by structure, substructure, name, synonym, partial name, and other text and numeric criteria. *ChemACX-SC* is a compilation of searchable catalogs from leading screening compound suppliers.

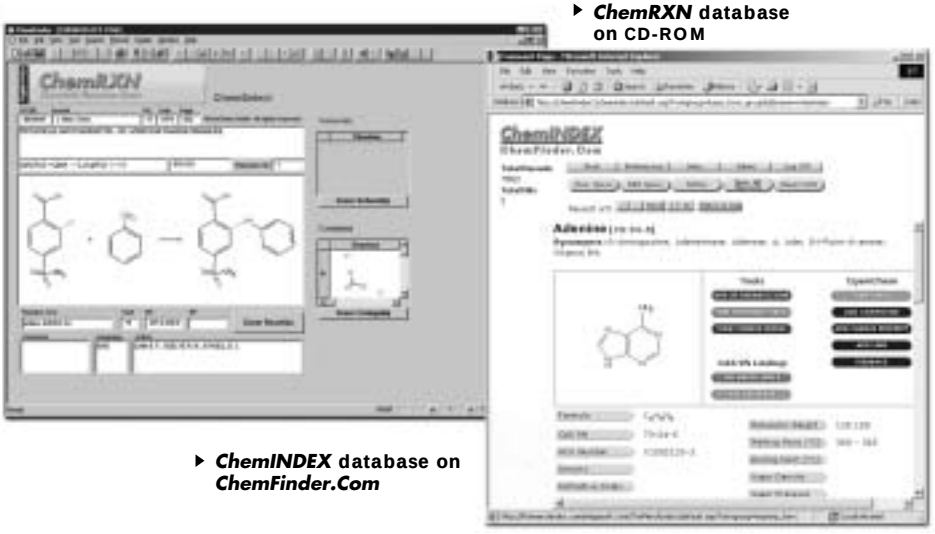
ChemACX.Com is the *ChemACX* web site with full search capabilities and convenient online ordering from major suppliers.

ChemINDEX includes 100,000 chemicals, public NCI compounds, and more.

ChemRXN is a collection of 30,000 fully atom-mapped reactions selected and refined from the chemical literature. It includes reactions from InfoChem's ChemSelect database and ISI's ChemPrep database.

ChemMSDX provides material safety data sheets for 7,000 pure compounds.

ChemFinder.Com is the award-winning web site with information and WWW links for over 100,000 chemicals. Search by name or partial name, view structure drawings, or use the *ChemDraw Plugin* for structure and substructure searches. View live *ChemDraw* files on Windows and Macintosh clients.



▸ ***ChemRXN*** **database on CD-ROM**

▸ ***ChemINDEX*** **database on *ChemFinder.Com***

SOFTWARE

The Merck Index
- Encyclopedic chemical reference

ChemACX Pro
- Chemical searching & buying

The Merck Index
Chemistry's Constant Companion
- Over 10,000 monographs of chemicals, drugs & biologicals

ChemACX Pro
Chemical Searching & Buying
- Database of commercially available chemicals: 300 catalogs with 500,000 chemical products
- *ChemACX-SC* database with 500,000 structures from leading screening compound suppliers

ChemACX.Com
WWW Chemical Searching & Buying
- Search by text, structure or substructure and order online from major catalogs

ChemINDEX
Reference Searching & Information
- NCI database of over 200,000 molecules, with anti-HIV & anti-cancer assay data

ChemRXN
Reaction Searching & Information
- Includes ChemSelect with reactions from InfoChem GmbH & ISI's ChemPrep

ChemMSDX
Safety Data Searching & Information
- Provides full Material Safety Data Sheets for over 7,000 pure compounds

ChemFinder.Com
WWW Reference Searching & Info
- WWW links for over 100,000 compounds
- Enter text queries or use *ChemDraw Plugin* for structure & substructure searching
- Works with Netscape & MS Internet Explorer

SYSTEMS & LANGUAGES

English & Japanese
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ChemOffice WebServer

Enterprise Solutions, Applications and Databases

ChemOffice WebServer

ChemOffice WebServer is the leading solution platform for enterprise, corporate intranet, and Internet scientific information applications. Compatible with major databases including Oracle, SQL Server, and Microsoft Access, *ChemOffice WebServer* is the development and deployment platform for custom applications and those listed below.

ChemOffice Browser

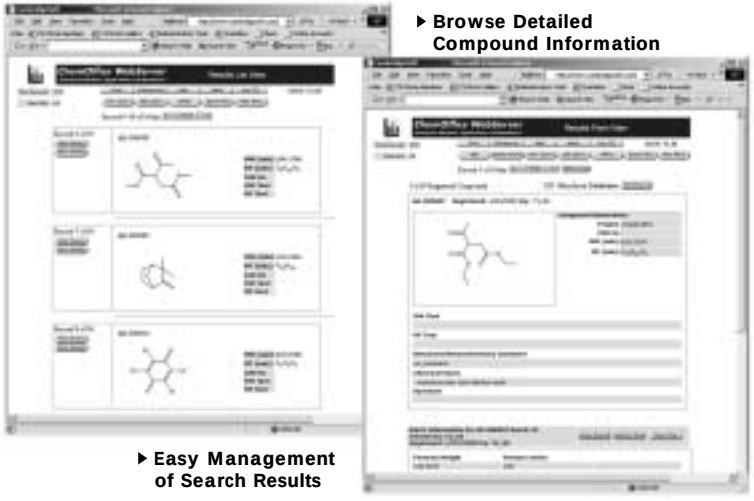
ChemOffice Browser, including *ChemDraw* Java, ActiveX, and the *ChemDraw* and *Chem3D Plugins*, brings the power and chemical intelligence of *ChemOffice* to Internet and intranet applications.

User Friendly & IT Ready

User-friendly and IT ready *ChemOffice WebServer* and *Browser* enterprise solutions, applications and databases are easier and faster for users to learn and the IT staff to deploy. Using *ChemOffice WebServer* technology, along with familiar browser technology, overall costs are lowered and less time is required for implementation.

Enterprise Solutions

Enterprise solutions built upon *ChemOffice WebServer,* including *Oracle Cartridge*, help workgroups and organizations collaborate and share information, just as *ChemOffice* supports the daily work of the scientist.



▸ **Browse Detailed Compound Information**

▸ **Easy Management of Search Results**

SOLUTIONS

- Development and deployment platform for workgroup and enterprise chemical information applications
- Webserver and browser components facilitate application deployment to desktops with minimal impact and training
- Enterprise Solution applications address areas of Knowledge Management, Research & Discovery, Applied BioInformatics and Chemical Databases

Knowledge Management

Knowledge Management applications organize and distribute chemical information. *E-Notebook Enterprise* streamlines daily record keeping with rigorous security and efficient archiving, and facilitates information retrieval by structure and text searching. *Document Manager* indexes the chemical structure content of documents, *Discovery LIMS* tracks laboratory requests, and *21CFR11 Compliance* implements an organization's regulatory compliance processes.

Research & Discovery

Research and discovery applications include *Registration System* for managing proprietary compound information, *Inventory Manager* for reagent tracking needs, and chemical databases for complete management of chemical inventories. *Formulations & Mixtures* and *CombiChem Enterprise* also provide tailored approaches to managing chemical data.

Applied BioInformatics

BioAssay HTS and *BioSAR Browser* applications process biological assay data to pinpoint the structural determinants of biological activity. *BioAssay HTS* supports low, high, and ultra-high throughput workflow, including sample and plate management, while *BioSAR Browser* probes structural details within assay data.

Chemical Databases

The Merck Index and *ChemACX Database* provide reference information, property estimations, and searchable compilations of commercially available chemicals.

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Oracle Cartridge

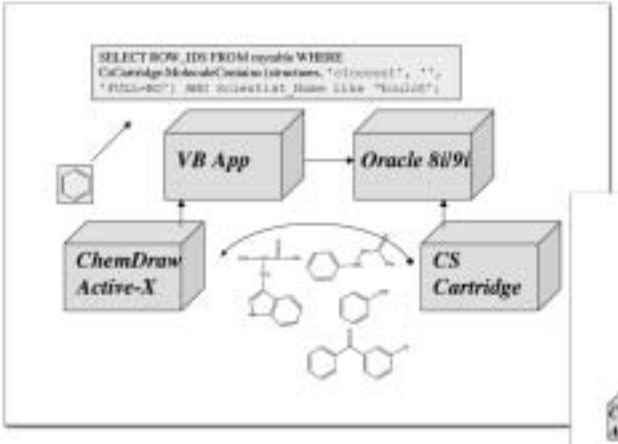
Enterprise Infrastructure for Database Security

WebServer Oracle Cartridge

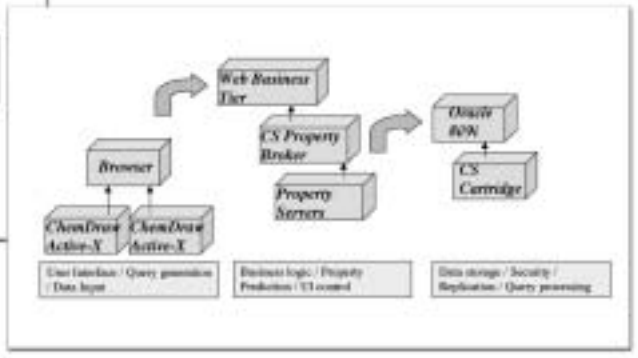
In scientific applications, the ability to store and manipulate chemical information is essential. By using CambridgeSoft's *Oracle Cartridge*, you add chemical knowledge to your Oracle platform and automatically take advantage of Oracle's security, scalability, and replication without any other external software or programs. You can search the chemical data by structure, substructure, and similarity, including options for stereo-selectivity, all through extensions to Oracle's native SQL language. Tools like PowerBuilder, Visual Basic and Visual C++ readily lend themselves as database clients. With the addition of the *ChemDraw* ActiveX control in the client, your end users can be structure-searching in no time.

Chemical Data Formats

CambridgeSoft recognizes that there is an enormous amount of legacy data out there in a myriad of formats, and most users have no desire to make wholesale changes to their chemical data generation or storage. To this end, *Oracle Cartridge* supports all major data types without translation or modification. In addition to CDX, it supports CDXML, MolFile, Rxn, and SMILES formats. Moreover, there are built-in extensions to SQL that allow you to extract data in all supported formats. Due to the variety of data formats supported, *Oracle Cartridge* is easily deployed even within existing applications. Since no manipulation of the data is needed, new records are automatically added to the index for searching.



▸ **Simple Client-Server Architecture**



▸ **Web Based Architecture**

- Adds chemical data types to Oracle, linking chemical applications to enterprise software systems without special programming
- Confers Oracle's security and scalability, simplifying large-systems' architectural considerations
- Makes legacy chemical data, such as MDL ISIS, accessible to *ChemOffice WebServer* applications

WebServer Enterprise Solutions

Even if you're not developing your own applications, or interested in the advanced data portability aspects of the *Oracle Cartridge*, CambridgeSoft's strategy will have a positive benefit for your IT infrastructure. CambridgeSoft's enterprise solutions are available in *Oracle Cartridge* versions, including *E-Notebook Enterprise*, *Document Manager, Registration System*, *Inventory Manager*, and *BioAssay HTS*. By utilizing *Oracle Cartridge*, you can deal with issues such as scalability and security entirely through the database layer, simplifying large-systems' architectural considerations. *Oracle Cartridge* has the side benefit of providing a database-level interface to key applications, so developers can integrate CambridgeSoft's solution platform with in-house IT solutions without tinkering with the business tier. Communicating with *Oracle Cartridge* is as simple as learning a few extensions to SQL.

Systems & Support

Support extends to include a variety of UNIX operating systems in addition to Windows servers. *Oracle Cartridge* has been deployed by large pharmaceutical companies with Oracle 8i and 9i.

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E-Notebook Enterprise

Desktop to Enterprise Knowledge Management

E-Notebook

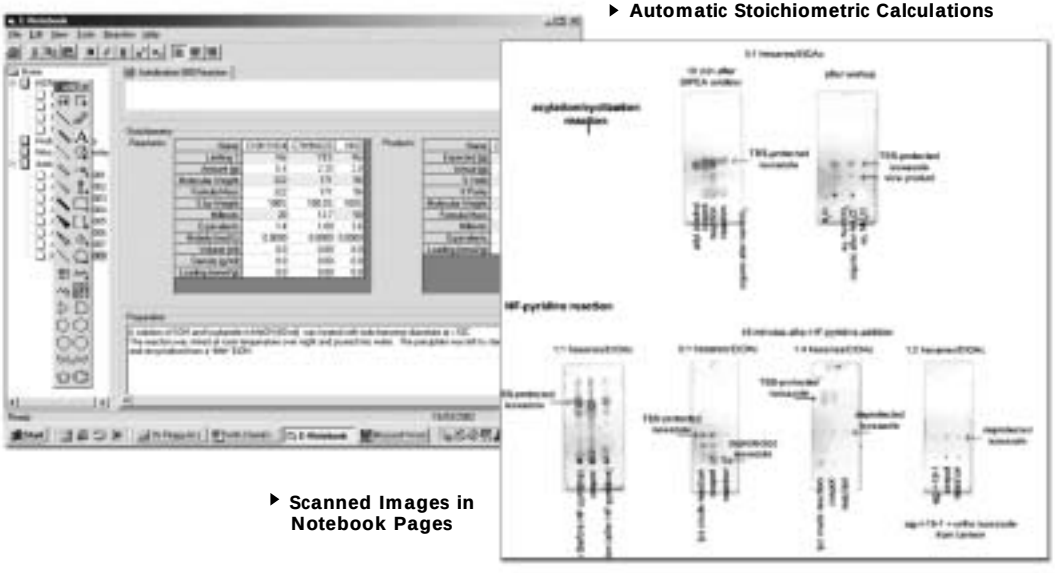
E-Notebook provides a smooth web-based interface designed to replace paper laboratory notebooks, with a fully configurable, secure system for organizing the flow of information generated by your organization. You can enter reactions, Microsoft Word documents, spectra and other types of data, and then search this data by text, substructure or meta-data. You can organize your electronic pages by projects, experiments or any other classification that conforms to your workflow.

Desktop to Enterprise

E-Notebook allows organization of notebook pages at either the personal or enterprise level. Enterprise groups can organize and store notebook pages in a central data repository, allowing colleagues to take advantage of each other's work. All access to data is subject to granular security. *E-Notebook* works with *Oracle Cartridge* and SQL Server, for departments or entire enterprises, and Microsoft Access, for individuals or small groups.

ChemDraw & Stoichiometry Calculations

While not quantum theory, stoichiometric calculations remain long and tedious. *E-Notebook* tackles this troublesome problem. First, draw your reaction directly in the page. Then, simply enter the mass, volume and den-



▸ Automatic Stoichiometric Calculations

▸ Scanned Images in Notebook Pages

- Custom organization of notebook pages at personal or enterprise levels with links to chemical registration
- Notebook pages include *ChemDraw* reaction schemes, Microsoft Word and Excel documents, and spectral data using the Galactic Spectral Control
- *Oracle Cartridge* provides detailed security and data integrity; SQL Server also available

sity, volume and molarity, and other factors of the limiting reagent and specify the number of equivalents of the other reactants. The notebook will do everything except calculate the experimental yield. To do that, you still have to run the experiment!

Microsoft Office & Galactic Spectra

E-Notebook manages all the other kinds of data chemists store in their notebooks. For free-form data, you can include Microsoft Word or Excel documents. For spectral data, you can take advantage of the Galactic Spectral Control embedded in the notebook that allows for analysis and storage of hundreds of kinds of spectra files.

Inventory Manager

E-Notebook includes an inventory of common reactants and reagents. If you have one of these common components loaded into the inventory application, all you have to do is click the *Add Reactant* button in *E-Notebook*. From here, you navigate to the desired compound and include it in your stoichiometry calculations. The enterprise edition of *E-Notebook* integrates with procurement and inventory management systems. Not only does this provide a useful way to know what compounds you have in stock and where they are located, it also saves time entering data.

Registration System

E-Notebook can be integrated into the entire chemical workflow of enterprise organizations. For example, once you record a reaction in your notebook, you can click a button to forward the products of the reaction to your compound registration system. These kinds of workflow enhancements increase productivity for the entire organization.

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Document Manager

Desktop to Enterprise Document Searching

Document Manager

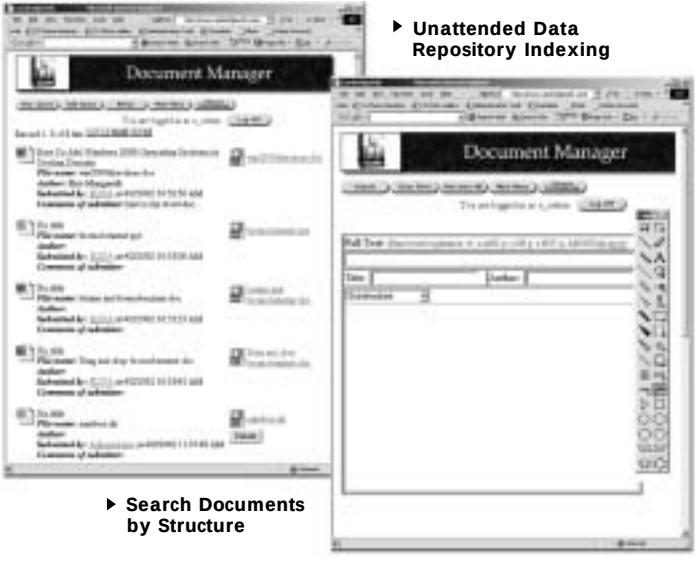
Everyone produces reports electronically, but searching information located in these reports has always been difficult. Thousands of Microsoft Word, Excel, PowerPoint, and other documents reside on file servers or individual computers, with no way to globally search them for information. Certainly, no easy way exists to search for the chemistry contained in these documents. *Document Manager* solves this problem, and requires no change in how you write and distribute reports.

Easy to Use

Document Manager manages a repository of new documents. These can be Microsoft Word, Excel, PowerPoint, or many other document types. When a new document is added, *Document Manager* automatically builds a free-text index of the document, and automatically extracts the chemical information into a chemically-aware, substructure searchable database. Chemical information can be both *ChemDraw* and ISIS/Draw. Finding information in reports is now as simple as entering a query through your web browser.

Unattended Data Indexing

As new documents are added they are automatically indexed and chemical information is extracted. Similarly, if a document is modified, it is re-indexed. No administration of the server is necessary other than routine back-up.



▸ **Unattended Data Repository Indexing**

▸ **Search Documents by Structure**

MANAGEMENT

- Indexes chemical structure information in documents and compiles a structure-searchable database
- Monitors designated folders or drives and automatically indexes new documents as they appear
- Documents are searchable by structure and free text

Free Text Searching

Documents are searchable by free text, including Boolean expressions, proximity operators, or simple queries. For example “author near Saunders” finds all Word documents where the word “author” appears near the word “Saunders”.

Advanced Chemical Searching

Since the chemical information is automatically extracted, documents can be queried by structure, substructure, similarity, molecular weight and formula. Chemical queries also support atom lists, Boolean operations on structures, superatoms, functional groups and many others. Queries can also be refined after an initial search, extending the power of the query language.

Structured Document Support

Structured documents, including documents created with Word templates or XML, are also supported. Information in structured documents is extracted and stored in specific fields of the database for more precise searching.

ChemFinder/Word

ChemFinder/Word, the desktop version, searches Word documents, Excel spreadsheets, *ChemDraw* files, *ChemFinder* databases, SD files, MDL molfiles, and more. Unlike other Microsoft Find facilities, *ChemFinder/Word* lets you work with the results you’ve located. Once you have a hit list, you can browse, search, refine, or export it to any destination.

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21CFR11 Compliance

Electronic Records and Signatures Regulations

The Challenge

Large and growing enterprises are facing a challenge to their core missions of developing and producing new products including food, therapeutic pharmaceuticals, medical devices, cosmetics or other health enhancing items. The complexity lies in complying with government regulations designed to protect public health and safety. The most notable of these is Title 21 of the Code of Federal Regulations governing Electronic Records and Signatures (21CFR11). Although 21CFR11 has been in the draft stage for almost a decade, final regulations have recently been created. Enforcement of these regulations is beginning to take place and enterprises are responding with a wide variety of initiatives, both within individual organizations and across industry sectors.

Integrated Software

CambridgeSoft applications, such as *E-Notebook Enterprise* and *Document Manager*, are at the leading edge of the integration of corporate knowledge management with *21CFR11 Compliance*. These products are designed so that as your organization reviews its internal processes for *21CFR11 Compliance*, the software can be configured to support these internal processes. Major requirements of 21CFR11, such as electronic signatures, audit trails, and long-term archiving, are incorporated within the routine workflow to generate the critical information required by research, development and production. In addition, *E-Notebook Enterprise* and *Document Manager* can be integrated with existing critical data systems.

▸ **Document and Record Management**

▸ ***E-Notebook* Data Capture**

- *E-Notebook Enterprise* and *Document Manager* integrate corporate knowledge with regulatory compliance
- Consulting teams analyze and adapt existing procedures to comply with new regulations
- Systems include authentication and digital signatures and adapt to changing regulations and demands

Analysis

As your enterprise develops the operating procedures that you will need to adopt for *21CFR11 Compliance*, CambridgeSoft's consulting team can provide invaluable assistance in analyzing your current operating procedures, adapting your existing procedures to comply with new regulations, and validating the software and the operating procedures that you will use. CambridgeSoft's consulting teams consist of individuals who have extended experience in deploying systems used by large pharmaceutical companies, emerging biotechs, and major enterprises worldwide.

Implementation

Once you have determined how your enterprise will comply with these new regulations, implementing those decisions needs to be done quickly, efficiently and with the understanding that the rules for compliance are in flux. In order to succeed, you must be able to respond to change. CambridgeSoft's *21CFR11 Compliance* consulting has both the tools and the expertise to provide complete solutions, carry out integration with your existing systems, and help you execute the process as quickly as your organization demands. Since ongoing monitoring is a part of business for regulated industries, you can be confident that, as regulations evolve and your requirements change, your systems can adapt. With CambridgeSoft, you can take advantage of the knowledge that has helped dozens of businesses, large and small, gain control over their business processes, their intellectual capital, and their material resources.

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Registration System

Chemical and Biological Registration

Registration System

Registration System includes a robust data model for pure compounds, batches, salt management, automatic duplicate checking and unique ID assignments. Compounds may be entered individually or with SD files. The data model resides entirely in Oracle and uses Oracle's security and transaction framework. For companies intending to modify or construct their own registration system, *ChemOffice WebServer* includes a powerful Software Developer's Kit (SDK) to add custom functionality. Instead of inventing a proprietary language, *ChemOffice WebServer* SDK extends the Microsoft and Oracle platforms, allowing information scientists to use the industry's most powerful development tools.

ChemDraw Plugin & WebServer

Registration System is easily adapted in almost any work environment. Its web-based, industry standard *ChemDraw* interface, makes *ChemOffice WebServer* the best choice for your corporate scientific information.

User Friendly Chemical Registration

New compounds are entered through a web form, and chemical, along with non-chemical, data is kept in a temporary storage area. When the compound is registered, it is compared for uniqueness via a configurable, stereoselective duplicate check, and assigned a registry number. All information about the compound, including its test data and other syntheses, is tracked by the registry number.

▸ Search for a Compound

▸ Display & Format Results

- Accessed through your favorite web browser, the system uses Oracle with robust data model to manage chemical products and their properties
- Checks for uniqueness during registration and optionally registers duplicates as batches of existing substance
- User administration and data entry are done through simple, easy-to-learn web forms; highly configurable system avoids tedious and expensive customization

Duplicate Checking with Override

When compounds are registered, the structure is checked for novelty. If a duplicate already exists in the database, the user can elect to register the information as a new batch of the existing compound, or assign it a unique registry number.

Oracle Cartridge

Registration System is the only true n-tiered application of its kind that is designed around thin clients and thin servers. This translates into ultimate flexibility on both the client and server side. Oracle is supported as a host, both with native security, on a variety of platforms and operating systems. The chemical information is directly stored in the Oracle tables.

Web Based User Interface

While the business logic of *Registration System* is complex, its user interface is clean and simple. Web browser support for Netscape Navigator and Internet Explorer, plus a choice of *ChemDraw Plugin*, *ActiveX* or *Java* client tools are provided. This significantly reduces training time and cost of client maintenance.

Advanced Chemistry Features

Duplicate checking is stereochemically aware. Batch data is maintained separately from compound data. Registration numbers support multiple sequences, including one for synthesized and one for procured. Compounds can be tracked by project and notebook reference, and registered in batches from SD files or other sources of molecular information.

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Inventory Manager

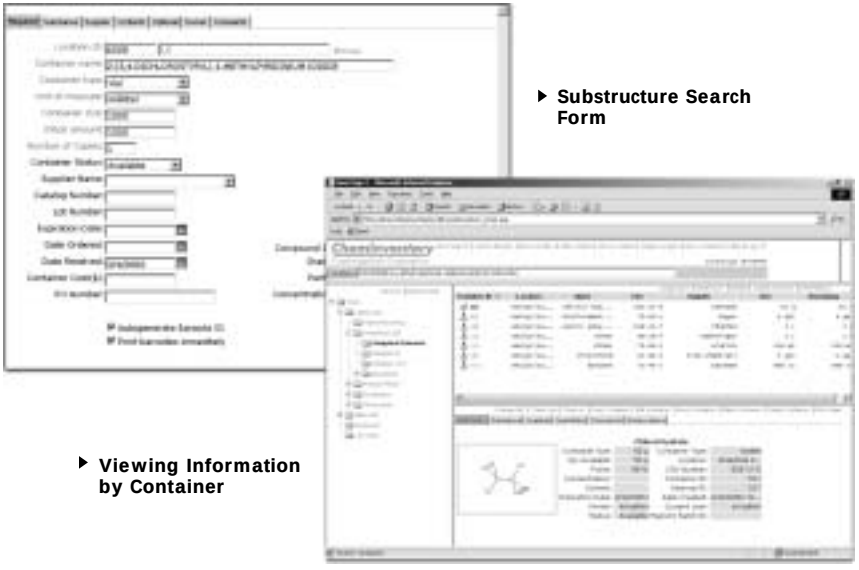
Chemical and Biological Inventory Integration

Database Technology

Inventory Manager is a *ChemOffice WebServer* based application designed to manage the reagent tracking needs of chemical and pharmaceutical research centers. The system manages data associated with both commercially and internally produced chemical substances. Although *Inventory Manager* is a stand-alone application, it can be tightly integrated with CambridgeSoft's *Registration System* and chemical procurement *ChemACX Database*. *Inventory Manager* is designed for a range of sizes from large workgroups to enterprises, and captures both stockroom and reagent needs as well as high-throughput discovery.

Cascading Location Model

Inventory Manager has a fully cascading location model. This means that laboratories can decide for themselves the granularity of their locations. Some labs may define locations as wells on plates residing on shelves inside refrigerators, which, in turn, are found in laboratories. Another lab may decide to track reagents at the bench or cabinet level. Still, in other settings, it may suffice to track chemicals on a lab-by-lab basis. The moving of chemical inventories is greatly helped by this model. For example, if an entire refrigerator is relocated, all of its containers move along with it. There is no need to re-catalog or reconcile, which saves a great deal of time.



▸ **Substructure Search Form**

▸ **Viewing Information by Container**

- Integrated with *Registration System* and *ChemACX* for procurement and life cycle chemical tracking
- Cascading location model allows different labs to track reagents at different levels (stockroom, refrigerators)
- Designed for tracking reagents, high-throughput discovery libraries, and true HTS plate management at multiple levels

Discovery, Reagents & Stockroom

Inventory Manager integrates fully with CambridgeSoft's *ChemACX Database* of available chemicals and *Registration System*. It also functions completely as a stand-alone application. Through this architecture, CambridgeSoft's enterprise solutions are truly plug-and-play. There are no added system integration costs, and the applications can live on different servers in different parts of the world.

Flexibility

The flexibility of the location model allows *Inventory Manager* to accommodate both reagent and discovery inventories in the same system. Each container in the system can be configured to track quantities in increasingly small values. A reagent bottle, for instance, can be measured as "full" or "empty", while wells in a 96-well plate can be measured in microliters. By moving such settings and preferences down to the container level, rather than system-wide or custom programming, *Inventory Manager* can accommodate both worlds in a single instance.

Integration with Purchasing & Registration

Inventory records are created directly from *ChemACX Database* of available chemicals, as well as from *Registration System*. For substances that do not exist in either database, *Inventory Manager* has its own chemically aware user interface. By tightly coupling with *ChemACX Database* and *Registration System*, the need for duplicate data entry is virtually eliminated. Once a product is ordered, its chemical information is stored and it is given an "on order" status, reducing duplicate ordering of popular reagents.

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CombiChem Enterprise

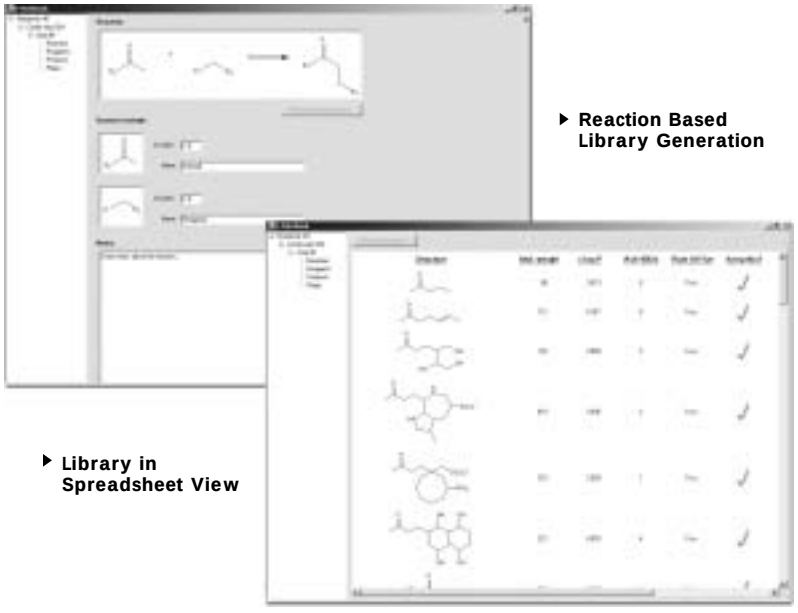
Desktop to Enterprise Combinatorial Chemistry

Benefits of Combinatorial Chemistry

Combinatorial chemistry, in particular the technique of parallel synthesis, has become an essential element of the drug discovery process. This is true both at the point of finding new leads as well as optimizing a promising lead. By using parallel synthesis techniques, chemists are able to multiply their productivity by a factor of between 5 and 100. This increase in productivity creates data management challenges. *CombiChem Enterprise* has been developed to provide the software tools required by the combinatorial chemist to manage and document parallel synthesis experiments. The software models real-world workflow as much as possible.

Starting Out

To start, the user simply draws a generic reaction step in a *ChemDraw* ActiveX control directly embedded in the notebook environment. Multiple reactants and products are supported. Points of variability on the molecules are indicated by the traditional "R" designation. Furthermore, query features can be used to precisely define the intended molecules. After drawing the reaction, the software analyzes the generic reaction, determines the role of each molecule, and creates pages for managing the lists of real reagents to be used in the actual parallel synthesis experiment.



▸ **Reaction Based Library Generation**

▸ **Library in Spreadsheet View**

- Reagent lists can be drawn from varied sources
- Reaction based library generation allows for evaluation by product or reagent
- Data management is simplified and library specifications are available to others on the network

Finding Reagents

Flexibility is the key when dealing with databases of chemical compounds. *CombiChem Enterprise* can use reagent lists from a variety of different sources: SD files, *ChemFinder* databases, *ChemFinder* hit lists, *ChemOffice WebServer* hit lists, *ChemACX Database*, or directly from the user via *ChemDraw*. Regardless of the source, *CombiChem Enterprise* produces a list of reagents which match a particular generic reactant. The chemist then chooses which of the compounds to use for generating products.

Getting Results

Once the chemist has given *CombiChem Enterprise* a set of reagents for each of the generic reactants in the reaction scheme, the software generates the set of products which would result from running the experiment. *CombiChem Enterprise* evaluates the products using several *in silico* methods, and the chemist can then choose which compounds to keep and which ones to reject. After the products have been generated, the software provides product information for each of the reagents. The chemist can use that information, for example, to trim away reagents having few or no products which pass the Lipinski Rule of Five test. Finally, the products are laid out on plates based on user-definable plate layouts.

Integration with *E-Notebook*

Keeping track of compound library data can be a challenge: which reagents led to this product, which product goes with that spectrum, what was in the mixture used in this thin layer chromatography? *CombiChem Enterprise* provides ways to organize the data and navigation is simple. When used with *E-Notebook Enterprise*, the data for a library of shared compounds, and the entire experiment, is automatically documented and made available to the entire organization.

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BioAssay HTS

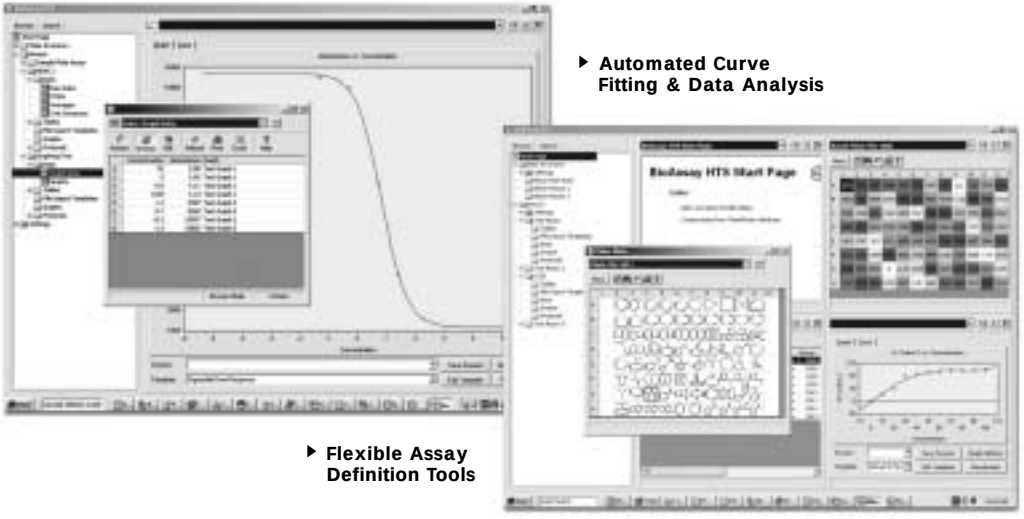
Biological Assay and High Throughput Screening

BioAssay HTS

BioAssay HTS provides scientists with an effective way of managing test results for biological and other kinds of experiments intended to assess the efficacy of compounds. Suitable for both plate-based high throughput screening assays and smaller-scale lead optimization experiments, *BioAssay HTS* provides researchers with simple tools for setting up their models in a database, uploading data, automating calculations and reporting on their findings.

User Friendly Assay Management

Even for the most basic protein assays, the independent and dependent variables used by the biologist to quantify efficacy can vary substantially from assay to assay. The underlying requirement that follows from this variability is for a flexible data management system that can adapt quickly to different assays and biological models. With *BioAssay HTS*, researchers or IT support staff simply define the observables and calculations that make up the assay. The database does the rest. Users can set up unlimited levels of drill-down. This allows users, for example, to click an IC50 and see a graph of percent inhibition versus concentration. Click again, and the software displays the original triplicate results, with outliers marked. The software even supports complex *in vivo* models.



- Effectively manages data from complex biological assays involved with lead optimization
- Adapts quickly and flexibly to different assays and biological models
- Closely integrated with Microsoft Excel, *ChemOffice* and *ChemDraw*

Easily Manage Large Volumes of Data

BioAssay HTS offers an easy way to capture large volumes of data from automated laboratory equipment and store it securely in Oracle. Scheduled data import means you can set up an import template once, and all future data will appear in the system as it is gathered. *BioAssay HTS* contains a complete plate inventory system that tracks plates and compound groups across plates. It easily manages daughter plate creation, barcoding, and freeze/thaw cycle tracking. Since it is integrated with your assay data, you can instantly view compound information and visualize results plate-wise to detect anomalies before they become a problem.

Automated Calculations & Curve Fitting

Once the database is configured for an assay, calculations are performed automatically whenever new data is entered or imported. Calculations can be quite complex, built from multi-step procedures. For an IC50 assay in triplicate, the software can average your triplicate results, take control values into account, and perform a sigmoidal dose-response curve fit according to your specifications. It is now as easy to do for 10,000 compounds as it is for ten.

Find Structure-Activity Relationships

Users can visualize data for multiple assays with *BioSAR Browser*, which is specifically designed for viewing structures and alphanumerics side-by-side. Other components of the *ChemOffice* product line provide additional ways to analyze structural and biological data and perform structure searches. Both *ChemFinder* and *ChemOffice WebServer* make it easy to create customized forms for viewing data. Users can export data to Excel or Spotfire for further analysis and reporting.

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BioSAR Browser

Biological and Chemical Meta Data Catalog

BioSAR Browser

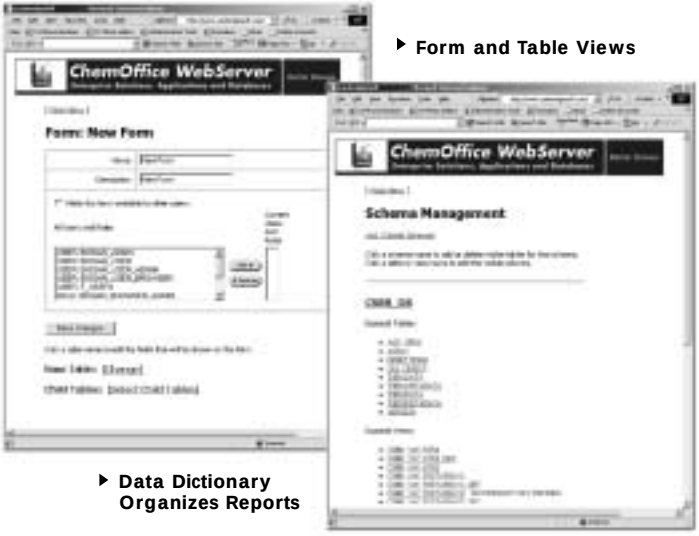
BioSAR Browser, a strategic must for any discovery organization interested in serious data mining, is a data-dictionary driven structure-activity analysis program. Users may choose among assays registered in the dictionary or search for assays of interest.

Providing Catalog Capabilities

The power of *BioSAR Browser* lies in the researcher's freedom from dependence on IT support. Once an assay is registered into the data-dictionary it is automatically included in the powerful analysis framework. By reducing the time between question and answer, *BioSAR Browser* gives researchers the freedom to explore new ideas—the bottom line for discovery information systems. Systems that provide answers after questions have become irrelevant are of no use. *BioSAR Browser* avoids this by placing application development in the researcher's control.

Forms & Tables in a Unified Interface

While most SAR tools provide only a table-based interface, *BioSAR Browser* provides a forms-based interface in addition to a tabular view. Researchers have demonstrated that both form and tabular views are essential. Forms provide highly detailed information about one compound, whereas tabular views make comparisons between



▸ **Form and Table Views**

▸ **Data Dictionary Organizes Reports**

- Catalog driven data mining and analysis operation
- Both form and table views available within simple web interface; *ChemDraw for Spotfire*
- Role based security specifies operations allowed for administrators, publishers and browsers

compounds more feasible. There is often a tradeoff between power and simplicity, and most SAR tools opt for the former at the expense of the latter. *BioSAR Browser*, however, merges the sophistication of a powerful data catalog technique with knowledge gained through years of working closely with users. The result is a SAR application that is as intuitive as it is powerful.

Security & Convenience

Security within *BioSAR Browser* is highly granular. Different roles exist for administrators, publishers, and browsers. Administrators may add assays to the data catalog engine, publishers may create reports and publish them, and browsers may use data query and analysis. Most data mining tools provide a mechanism to store queries, but the interface for creating queries is too complex. With *BioSAR Browser*, each set of assays is a complete report with a query form, a view form, and a table view, combining the convenience of a *ChemFinder* or ISIS application with the power and flexibility of a data catalog-driven mining program.

ChemDraw for Spotfire

ChemDraw for Spotfire is a powerful add-in for the Spotfire DecisionSite software. Spotfire makes industry standard applications for high-dimensional visual data analysis, and is used to explore large biological datasets. *ChemDraw for Spotfire* adds chemistry to DecisionSite, providing structure visualization and searching services. Highlight a spot in Spotfire's DecisionSite, and a structure is displayed directly in the window. If you draw a structure and click *Search*, the matching records are displayed right in the Spotfire window. The structures are retrieved from a chemical database such as *Registration System*, *ChemFinder*, or *Oracle Cartridge*, and are returned directly over the network. In this way, structures can be linked by registry number, CAS number, or

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ChemACX Database

Available Chemicals and Screening Compounds

ChemACX Database

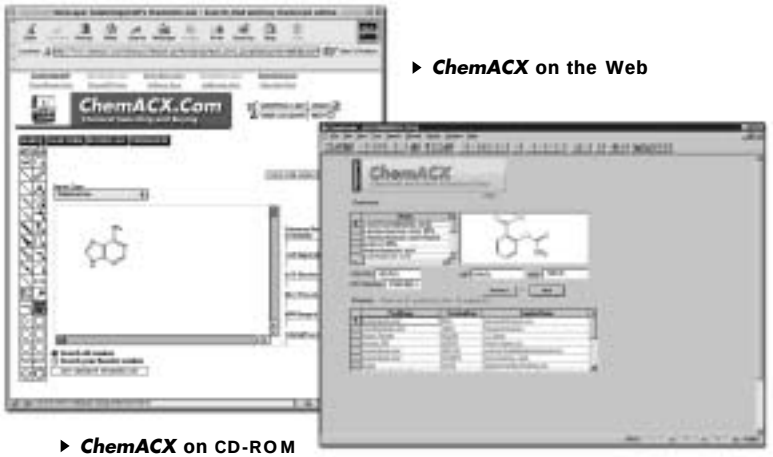
Sifting through chemical catalogs is a poor use of time for any researcher. The Available Chemicals Xchange database, *ChemACX Database*, provides a complete tool for research chemical sourcing and purchasing. The database can be accessed from both desktop and enterprise environments and boasts an impressive list of major suppliers, from Alfa Aesar and Aldrich, to TCI and Zeneca with hundreds in between. The enterprise procurement solution for *ChemACX* saves time by streamlining the entire purchasing process. Use *ChemACX* to build an internal requisition, print the form on your company template, fill it out and submit it to purchasing.

ChemACX-SC

ChemACX-SC is an additional fully structure searchable database containing the catalogs of leading screening compound suppliers, including ChemBridge, Maybridge, Sigma-Aldrich's Rare Chemical Library and others.

Data Quality

Over 500,000 products from 300 research chemical and biological catalogs have been selected to have their product catalogs prepared for electronic delivery. The data provided by the suppliers is enriched by editors who add searchable chemical structures, physical and chemical properties, and incorporate a comprehensive chemical synonym dictionary. All substances and supplier catalog numbers are cross-referenced, making it easy to locate alternate sources for back ordered or discontinued items.



▸ ***ChemACX* on the Web**

▸ ***ChemACX* on CD-ROM**

- Fully structure-searchable database of 500,000 products from 300 chemical catalogs; separate *ChemACX-SC* database contains screening compounds
- Search by name, synonym, partial name, formula, and other criteria, as well as structure and substructure
- Shopping cart system works with requisition forms and purchasing systems, such as SAP, Ariba and Commerce1, to streamline chemical purchasing

Data Currency

A premium is placed on the accuracy and currency of the *ChemACX Database*. Many suppliers listed in the database are also currently selling their products online through the *ChemACX.Com* web site, and therefore have a vested interest in ensuring that their data remains complete, accurate and up-to-date. You won't find a sourcing database with more frequently updated content and current pricing than *ChemACX*.

Data Accessibility

The same way that Internet users can publicly access *ChemACX.Com*, enterprise users can access their private *ChemACX Database* via a standard web browser. There is no need to configure or install any additional software. *ChemDraw* users can either use the *ChemDraw Plugin* to draw chemical structures directly in the browser's search page, or alternatively submit queries to the database server directly from *ChemDraw*. *ChemFinder* users can access their own copy of the database right from their local hard drive.

Electronic Requisitions

Traditional sourcing databases were conceived merely as reference tools. *ChemACX Database*, however, goes one step further by including the ability to collect products into an electronic shopping cart and export its contents into electronic requisition forms or purchasing systems. This time-saving feature has proven to be one of the most popular advantages of *ChemACX* among scientists and purchasing agents alike. Users can readily export data from the shopping cart into Excel and Word templates used as departmental requisition forms.

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The Merck Index

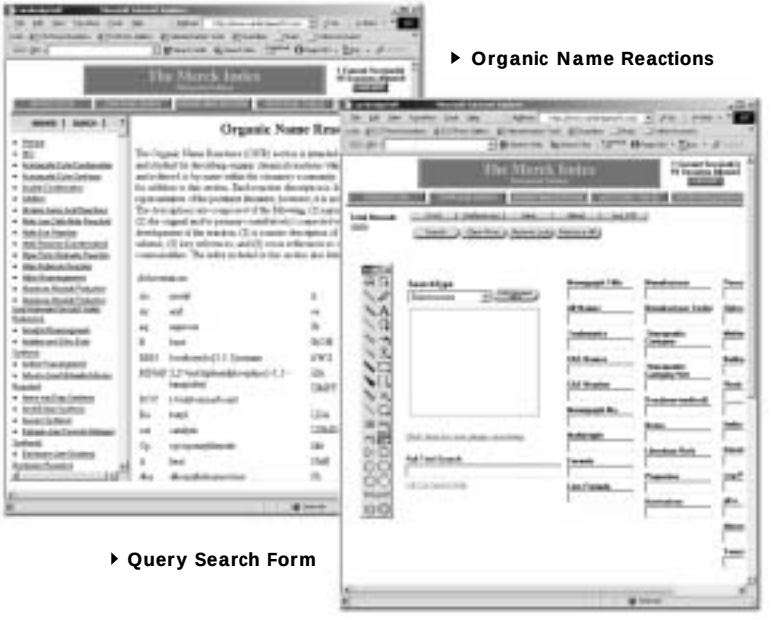
Chemistry's Constant Companion

Industry Standard

Among printed chemical reference works, one that stands out for its integrity, detail and longevity is *The Merck Index*. This encyclopedia of chemicals, drugs and biologicals has 10,250 monographs, 446 named reactions and 23 additional tables. Merck & Co., Inc., the publisher of *The Merck Index*, has chosen CambridgeSoft to produce the complete contents of the 13th edition in a fully searchable *ChemOffice* format.

Detailed Monographs

The subjects covered include human and veterinary drugs, biologicals and natural products, agricultural chemicals, industrial and laboratory chemicals, and environmentally significant compounds. What makes *The Merck Index* so valuable is its extensive coverage. The information provided includes chemical, common and generic names, trademarks, CAS registry numbers, molecular formulas and weights, physical and toxicity data, therapeutic and commercial uses, and literature citations. In addition to the standard searches, compound monographs can now be searched by *ChemDraw* structure as well as substructure. Moving this information to the fully searchable *ChemOffice* format makes it easier and faster to search and get results. Instead of consulting the auxiliary indices and then turning to the actual monograph, all searching can be done from a single form.



▸ Organic Name Reactions

▸ Query Search Form

- Encyclopedic reference for over 10,000 chemicals, drugs, and biologicals
- Fully searchable by *ChemDraw* structure, substructure, names, partial names, synonyms and other data fields
- Available in desktop, enterprise and online formats

Integrated Information

Having *The Merck Index* in *ChemOffice* format confers another valuable benefit: integration with other information sources. For example, after locating a substance in *The Merck Index*, it is a simple matter to copy the name, structure or other data elements to search *ChemACX Database* to find out whether there are commercial suppliers of the substance. The structures could also be used as input to *Chem3D* to obtain three-dimensional models and to perform electronic structure and physical property calculations. Information can also be brought into any *ChemOffice* desktop or enterprise solution, including *ChemDraw/Excel*, *ChemFinder/Word*, *E-Notebook* and *Registration System*.

ChemOffice Formats

The Merck Index is available in two *ChemOffice* compatible formats. The desktop edition is a CD-ROM in a *ChemFinder* database format, for use by an individual researcher. The enterprise edition, designed for workgroups and larger user communities, is served by *ChemOffice WebServer* to connected users. *The Merck Index* thus adds to the growing set of reference databases served by *ChemOffice WebServer*. Just as *ChemOffice* integrates the desktop edition of *The Merck Index* with the scientist's everyday activities, the enterprise edition becomes an integral part of the applications deployed on *ChemOffice WebServer*.

Web Versions

The complete contents of *The Merck Index* are also available online through your favorite web browser. To meet your specific needs, single user subscriptions, corporate extranet subscriptions and intranet webservers are all available.

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Chemical Databases

Reference, Chemicals, Reactions, Patents and MSDS

Databases

ChemOffice WebServer provides a full range of compound and reaction databases essential for research. Databases are available at *ChemFinder.Com*, or over corporate intranets.

Reference

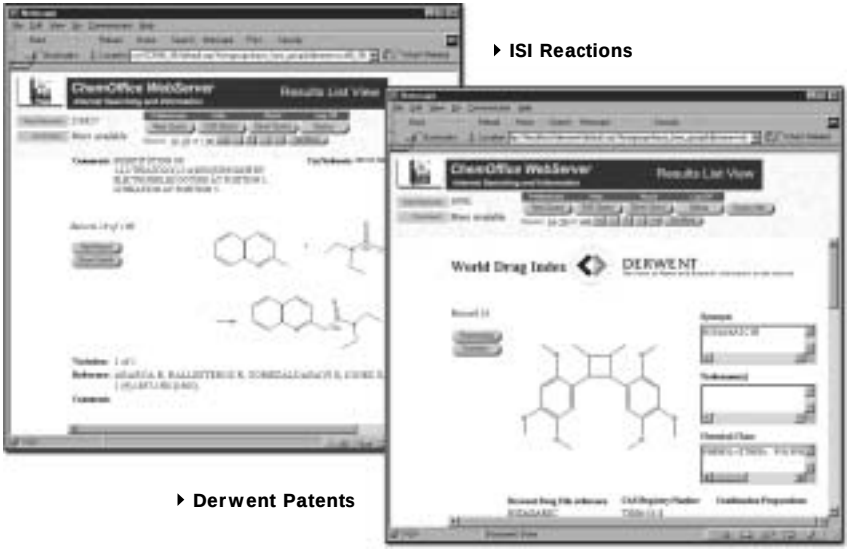
The Merck Index contains encyclopedic references for over 10,000 chemicals, drugs and biologicals.

ChemINDEX includes 100,000 chemicals, public NCI compounds and others.

World Drug Index (WDI) from Derwent contains over 58,000 compounds with known biological activity. WDI classifies compounds according to type of biological activity, mechanism, synonyms, trade names, references and more.

Chemicals

ChemACX and ***ChemACX-SC***, Available Chemicals Xchange, is a large and growing source for information on compound availability. It lists compounds from Alfa Aesar and Aldrich to TCI and Zeneca with hundreds in between, including 500,000 products from 300 catalogs. *ChemACX-SC* is a library of screening compounds.



- Extensive collection of chemical reference information in fully searchable database format
- Includes information on commercial availability; properties; biological activity; organic reactions; material safety data sheets; and patent or development status
- Developed by CambridgeSoft in partnership with the leading chemical database publishers

Reactions

Organic Syntheses is the electronic version of the annual and collective volumes of trusted, peer reviewed synthesis procedures published since 1921 by Organic Syntheses.

Current Chemical Reactions (CCR) from ISI is both a current awareness and a data mining application used to design chemical syntheses. Renowned for its quality, CCR contains information from over 300,000 articles reporting the complete synthesis of molecules. Updated daily, CCR is an excellent way to stay on top of recent developments.

ChemReact and **ChemSynth** from InfoChem are carefully selected from a database of over 2.5 million reactions through an automated process of reaction classification. With over 390,000 reaction types, ChemReact is for expert synthetic chemists designing novel syntheses. Entries in ChemSynth are further refined to those with over 50% yield and at least two literature references.

ChemRXN is a refined selection of over 29,000 fully atom-mapped reactions. Including carefully selected reactions from InfoChem's ChemSelect database and ISI's ChemPrep database, *ChemRXN* is a terrific combination of utility.

Patents

World Drug Alerts (WDA) from Derwent is a current awareness application providing information on patents, new biologically active compounds, new methods for synthesizing drugs, and other data. It is a requirement for effective decision making in all stages of drug design.

Investigational Drugs Database (ID db) from Current Drugs is the world's leading competitor intelligence service on drug R&D. Updated weekly, it covers all aspects of drug development world wide, from first patent to launch or discontinuation.

Safety MSDS

ChemMSDX provides over 7,000 material safety datasheets.

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Consulting & Services

Development, Installation & Training Services

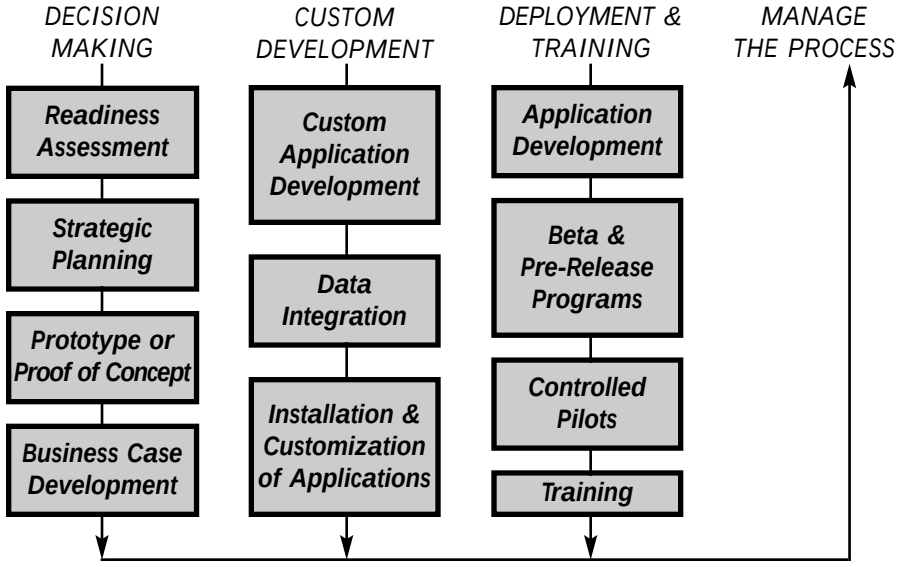
Managing Information

Today's businesses are facing many complex issues. Among them are the overloads of disparate types of information, unmanaged proliferation of valuable research data, virtual projects in many locations, uncontrolled research data, compliance, certification and regulation. Technological solutions to these issues require careful planning and management. CambridgeSoft now offers the following professional services to assist businesses in fully utilizing the power of technology.

Decision Making

CambridgeSoft believes that successful technology utilization begins with the assessment and decision making process. Our experts can assist clients with:

- *Readiness Assessment*: Identify the scope, requirements, and deliverables for your project. Assure critical IP is incorporated. Allow end-users to capitalize on existing scientific and technology resources.
- *Strategic Planning*: Conduct formal analysis of scientific, technical, operational, and process environments to determine the necessary approach to customization and deployment.
- *Prototypes and Proof of Concept*: Prototypes allow you to test the technical feasibility of solutions. This activity can provide a baseline for the future roll-out of the solution, and can also gather user feedback so requirements can be refined.



- *Business Case Development*: Business cases help define a clear and purposeful solution based on well-defined and documented business needs. Having a business case helps to justify good projects, stop bad projects before they are started, and provides the basis for ongoing measurements after project completion to make sure that the business is getting the results they wanted.
- *Operational Planning*: In order to effect change on complex environments, it is necessary for organizations to develop operational plans. These plans minimize the risks associated with large technology deployments. Plans may incorporate key business processes and workflows, and help to identify any operational constraints.

Custom Development

Your organization requires solutions that meet you unique needs. CambridgeSoft consultants can assist with:

- *Custom Application Development*: Assess business needs, document specifications, and create custom web-based solutions for your enterprise.
- *Data Integration*: Create interfaces with other data management systems to incorporate your data into an enterprise system.
- *Installation and Customization*: Customize your solution to your specifications. Make certain that all technical and logistical installation processes are managed.

Deployment & Training

Develop a comprehensive road map for deployment of technology solutions across the enterprise. Our experts help you plan and deploy your solutions by:

- *Application Deployment*: Document, define and execute all of the actions required to support end user acceptance. Manage the deployment process to assure a smooth roll-out to the end-users
- *Beta and Pre-Release Programs*: Beta and pre-release programs involve a limited deployment to a small set of users in order to identify deployment readiness or logistical issues that must be addressed prior to a large-scale deployment. When early release programs are employed, the success rate of large scale deployments is greatly increased and end users are more likely to adopt the new technology.
- *Controlled Pilots*: Controlled pilots involve deploying a pre-production system to a small group of users to evaluate it's functional, usability, technical, and operational characteristics in a real-world environment prior to the completion of final system development. A controlled pilot helps identify and correct show-stopper technology or operational issues before a final roll out program is implemented.
- *Training*: Develop customized training materials for users, system administrators, and help desk personnel. If you choose to outsource training management, CambridgeSoft can schedule and conduct training for all users and stakeholders.

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CS Software Problem Report

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USER INFORMATION (Please Print Legibly)

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Title _____

Firm _____

Street _____

City _____ State _____ Zip _____

Country _____

Tel _____ Fax _____

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DETAILS OF THE PROBLEM

SYSTEM CONFIGURATION

SOFTWARE

Application Name _____

Version Number _____

Serial Number _____

SYSTEM

Windows (version) _____

MacOs (version) _____

Web Browser(s) (version) _____

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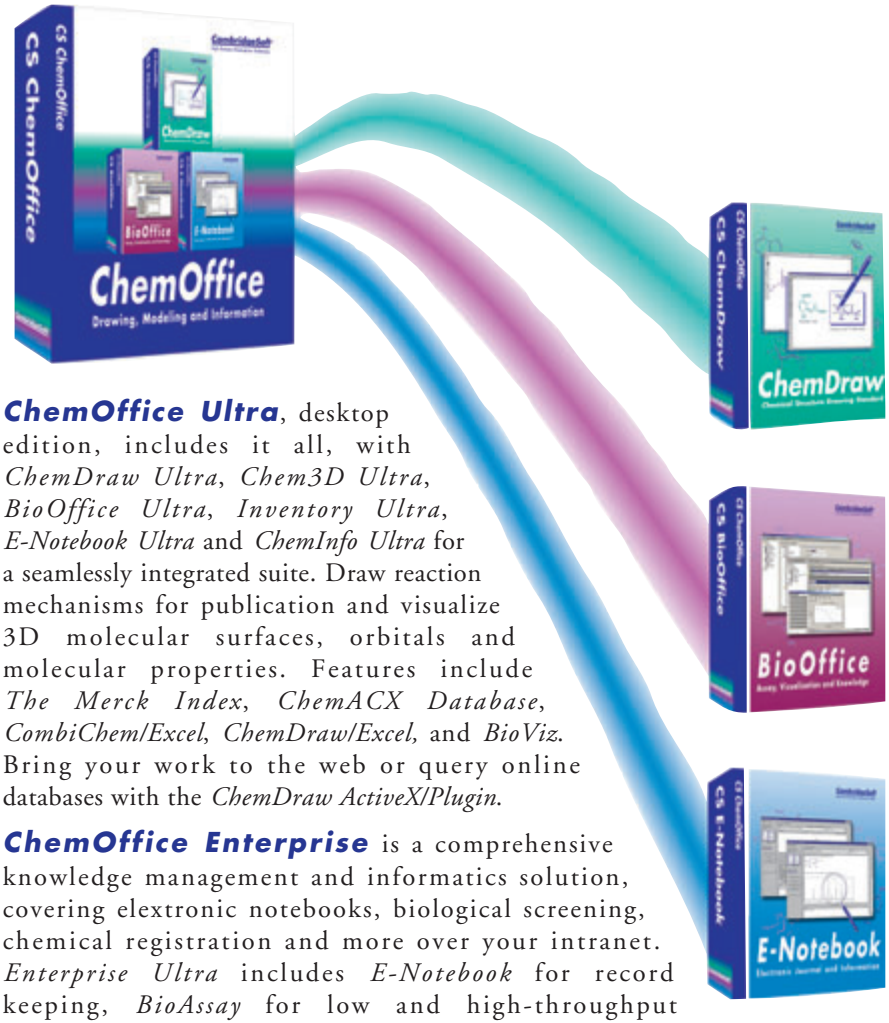

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